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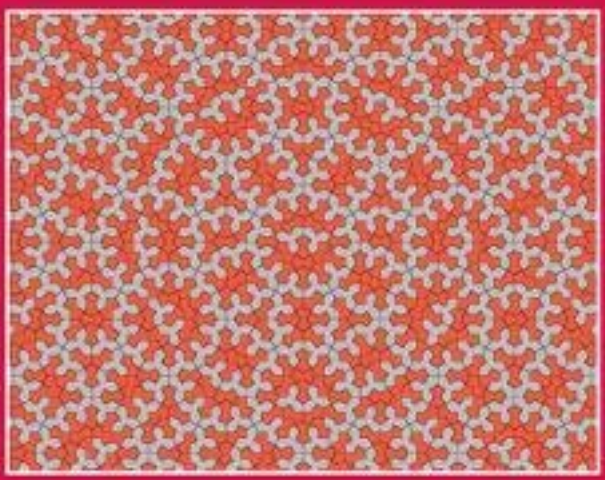
APERIODIC ORDER

Volume 2: Crystallography and Almost Periodicity

Edited by
Michael Baake and Uwe Grimm



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APERIODIC ORDER
Volume 2: Crystallography and Almost Periodicity

Quasicrystals are non-periodic solids that were discovered in 1982 by Dan Shechtman, Nobel Laureate in Chemistry 2011. The mathematics that underlies this discovery or was stimulated by it, which is known as the theory of Aperiodic Order, is the subject of this comprehensive multi-volume series.

This second volume begins to develop the theory in more depth. A collection of leading experts in the field, among them Robert V. Moody, introduce and review important aspects of this rapidly-expanding field.

The volume covers various aspects of crystallography, generalising appropriately from the classical case to the setting of aperiodically ordered structures. A strong focus is placed upon almost periodicity, a central concept of crystallography that captures the coherent repetition of local motifs or patterns, and its close links to Fourier analysis, which is one of the main tools available to characterise such structures. The book opens with a foreword by Jeffrey C. Lagarias on the wider mathematical perspective and closes with an epilogue on the emergence of quasicrystals from the point of view of physical sciences, written by Peter Kramer, one of the founders of the field on the side of theoretical and mathematical physics.

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ENCYCLOPEDIA OF MATHEMATICS AND ITS APPLICATIONS

Aperiodic Order

Volume 2: Crystallography and Almost Periodicity

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Foreword by Jeffrey C. Lagarias

The mathematical study of aperiodically ordered structures is a beautiful synthesis of geometry, analysis, algebra and number theory. On the mathematical side, it arose in connection with tilings as a model of computation (the undecidability of the domino problem of Hao Wang) and the existence of ever simpler aperiodic tilings, exemplified by the Penrose tiling. From the physics side, it received great impetus from the discovery of Dan Schechtman in 1982 (published in 1984, Nobel Prize in Chemistry 2011) of an AlMn alloy whose X-ray diffraction spectrum exhibited long-range order of atomic positions and spacings with icosahedral symmetry.[1] That is, the sample exhibited an X-ray diffraction pattern with sharp spots with 10-fold, 6-fold and 2-fold symmetries when rotated to the corresponding directions of the icosahedron. Such a symmetry is incompatible with the material having an atomic structure that is periodic in any direction.

This discovery raised several questions, such as:

(1) Do ideal structures exist that have diffraction spectra with sharp spots and (perfect) non-crystallographic symmetries?

(2) Are there 'local conditions' permitting or favouring the assembly of such structures?

These two questions received positive answers in the 1980s, in the sense of mathematical constructions which achieve all or most of them. One such construction leads to cut and project sets and so-called model sets, which are described in detail in the first volume of this series [AO1]. There was earlier theoretical work anticipating these structures by various people, including Mackay (1981), Kramer (1982) as well as Kramer and Neri (1984).

There remain serious mathematical problems in extending these answers to a larger range of validity, including:

(i) Construction of interesting point sets;

(ii) Determination of local (matching) rules to force aperiodicity;

(iii) Classification of the possible types of symmetry.

[1] The corresponding references can be found in the bibliography of the first volume in this series [AO1]. Selected additional or new references will be given explicitly.

Answering these questions motivated the development of an extension of classical crystallography that is suitable to describe such structures, nowadays known as quasicrystals. In addition, establishing new notions of 'equivalence' of (aperiodic) structures requires new concepts. For instance, this task led to developments in ergodic theory with larger group actions, such as $\mathbb{Z}^d$, $\mathbb{R}^d$, or the Euclidean isometry group $\mathbb{R}^d \rtimes \mathrm{O}(d)$.

Besides the two questions above, there is a third question, concerning the inverse problem of reconstructing information on the atomic structure from diffraction data or from scanning tunneling electron microscope data. This amounts to asking: 'Where are the atoms?', which still seems a difficult problem to handle.

There are two major types of structures studied in aperiodic order. The first type consists of *Delone set models*, which concern uniformly discrete sets of points modelling the solid state, often imposing restrictions on allowable interpoint distance vectors. The second type consists of *tiling models*, where one studies tilings of Euclidean space with a finite number of distinct tile shapes, often polyhedra. In some of these models, additional 'matching rules' are imposed on how tiles may be placed next to each other. There are methods for taking a model structure of one type and converting it to the other type. For Delone sets, one may associate to it the tiling of space given by the Voronoi cells around its points. For a tiling model, one may mark a few points in the interior of each tile to assign a Delone set to the tiling.

Generalisation of geometric crystallography

The subject of *geometric crystallography* [5] was developed in the 19th century. Based on atomistic concepts, it considered infinitely extended discrete sets of points Λ in space $\mathbb{R}^d$, called *regular point systems*, which are discrete sets that 'look the same' when centred at any point in them. That is, the set Λ is preserved by any translation mapping one point of it to any other. A foundational result is that any such system of points must form a single (full-dimensional) lattice Γ of points in $\mathbb{R}^d$. One may then classify such systems according to their full set of Euclidean symmetries (allowing reflections). This was accomplished for two dimensions in the 1870s and in three dimensions in independent work of Federov (1891), Schoenflies (1893) and Barlow (1893).

The problem of establishing a finite classification in d dimensions was raised by Hilbert in 1900 as part of his 18th problem. The first step to its solution was contributed by Bieberbach, who by 1912 showed that there are only finitely many symmetry types in each dimension. The classification in four dimensions was completed in 1978 by Brown, Bülow, Neubüser, Wondratschek and Zassenhaus.

A generalisation of regular point systems is that of *multiregular point systems*. These are infinitely extended discrete sets in $\mathbb{R}^d$ which, when centred at any point, are isometric to one of a finite list of such systems (fixing a marked centre point). Dolbilin et al. [3] showed that any such system necessarily is the union of a finite number of translates of a full-dimensional lattice Γ, so is fully periodic (or crystallographic).

To allow aperiodic point patterns, one enlarges the set of crystallographic point sets to Delone sets, or (r, R) sets, which are infinitely extended sets such that no two points are closer than distance r and such that each ball of radius R contains at least one point. There is a useful taxonomy on Delone sets that nicely extends the framework of geometric crystallography.

The first idea is to generalise the notion of regular point system to require the agreement of patches of a finite radius, rather than all the way to infinity. For a fixed set Λ, a patch of radius T centred at $x \in \Lambda$ is the set $\Lambda \cap (B_T(0) + x)$. In 1976, Delone and coworkers showed that regular point systems could be characterised by the property that they locally 'look the same' when centred around each point out to a sufficiently large finite radius T, where T is a function only of the Delone set parameters (r, R) and the dimension d. An extension of this result holds for multiregular point systems as well: If $\Lambda \subset \mathbb{R}^d$ is a Delone set that has exactly k different isometry classes of centred patches of a given radius T, with T sufficiently large with respect to k, namely $T \geqslant CRk$ with $C = 2(d^2+1)\log_2(2(R/r)+2)$, then Λ is a multiregular point system having k different isometry classes of (infinite radius) patch types [3].

The second idea is to restrict the allowable interpoint distance vectors. The class of *finite local complexity* (FLC) Delone sets comprises those Delone sets Λ for which $\Lambda - \Lambda$ is a discrete and closed set. In fact, it suffices to check this condition out to a finite radius $2R$: One only needs that $(\Lambda - \Lambda) \cap B_{2R}(0)$ is a finite set. One consequence is that the points of FLC Delone sets can be labelled by 'coordinates' in a finite-dimensional module, embedded in a space of dimension higher than that of the ambient space of the Delone set.

To go one step further, one considers *Meyer sets* in $\mathbb{R}^d$, which form the subclass of Delone sets Λ for which the interpoint distance set (or Minkowski difference) $\Lambda - \Lambda$ is a Delone set. This version has been shown to be equivalent to Meyer's original notion [11], which is that of relatively dense sets Λ such that $\Lambda - \Lambda \subseteq \Lambda + F$ with F a finite set.

A quantification of order for FLC Delone sets is provided by numerical combinatorial invariants of the structure of their finite patches. The *patch-counting function* $f(R)$ counts the number of translation-inequivalent patches of radius R. The growth rate of this function with increasing R is a combinatorial measure of the possible kind of order. It has been shown by Lagarias

and Pleasants (2002) that, if this growth rate is sublinear, the function must be eventually constant and the structure must then be an ideal crystal. A second quantifier concerns measures of distances for the repetition of different patches of large radius in the set. One says that an FLC Delone set Λ is *linearly repetitive* if there is a constant C such that every fixed patch of radius ρ that occurs somewhere in the set necessarily occurs within distance $C\rho$ of any point of Λ. This condition holds for Penrose tilings, for example, and it also implies that such a set must have a well-defined diffraction measure.

Inflation rules

A frequently used construction for aperiodic patterns employs structures that are (possibly approximately) preserved under an inflation operation. Meyer's work in harmonic analysis from the early 1970s included a study of discrete systems which may, in special cases, be preserved under an inflation rule, which reproduces a structure on a larger scale. He noted a connection between allowable inflation scales on these structures and algebraic numbers.

A point set Λ has an *inflation* if there is a number $\eta > 1$ such that $\eta\Lambda \subset \Lambda$; we call any such η an *inflation factor* for Λ. Meyer [12] proved for the sets which are now called Meyer sets that the inflation factor must be an algebraic integer which is either a Pisot–Vijayaraghavan (PV) number (all algebraic conjugates satisfy $|\eta'| < 1$) or a Salem number (all $|\eta'| \leqslant 1$ and some $|\eta'| = 1$). The golden ratio $\tau = \frac{1+\sqrt{5}}{2}$ is a PV number. It features in the mathematics of the icosahedron and appears in all tiling models with icosahedral symmetry as well as in fivefold symmetric tilings of the plane. Later, in 1999, I observed that there is also an algebraic restriction on inflation factors $\eta > 1$ of FLC Delone sets: They must be real algebraic integers all of whose algebraic conjugates η' satisfy $|\eta'| \leqslant \eta$.

Packing problems and quasicrystallinity

Packing problems have been observed to possess connections with crystallography. The general packing problem includes the determination of the densest packings attainable by identical copies of fixed solid geometric objects, particularly convex bodies. Minkowski's 'Geometry of Numbers' concerns the problem of finding the densest lattice packing of identical copies of a given convex body, movable by translations only. Allowing rotations of the body, as in the case of tetrahedra, leads to new problems.

Notable examples have densest packings attainable by a crystalline structure. For equal spheres, the densest packing in dimensions up to three are all attained by lattice packings. In three dimensions, there are also equally

dense periodic packings of various types, as well as packings that are aperiodically stacked in one direction while being periodic in the two independent directions orthogonal to it.

Recent developments suggest that suitable tiling questions may also lead to quasicrystalline structures. For packings of regular tetrahedra, there are no mathematical proofs but there are results obtained by simulation. The densest known packing of regular tetrahedra has a periodic structure with four tetrahedra in the unit cell [2]. On the other hand, Monte Carlo simulations of Haj-Akbari and coworkers [6] of a 'gas' of regular tetrahedra at high pressure (meaning ensembles having density close to this maximal value) suggest they have a quasicrystalline structure in two directions, while having a periodic structure in the third direction. Specifically, samples displayed a diffraction pattern (for point scatterers located at centroids of the tetrahedra) that exhibits a ring of peaks indicating a 12-fold symmetry.

Diffractivity

The study of diffractivity properties of aperiodic sets requires Fourier analysis and distribution theory. Here, we only consider diffraction for point sets in $\mathbb{R}^d$, although Meyer — and later Moody as well as Schlottmann — have shown that the analysis of diffraction can profitably be done in the more general setting of locally compact Abelian groups. The formulation of a general mathematical notion of diffractivity suitable for diffraction of aperiodic sets (via a connection with ergodic theory) was initiated by Dworkin (1993) and extended by Hof (1995). It uses a framework of locally finite measures, which for $\mathbb{R}^d$ can be viewed as a subclass of tempered distributions. An autocorrelation measure is associated to a given spatial distribution of δ-functions as a locally finite measure; see [AO1, Chs. 8 and 9] for a detailed exposition. The diffraction data is the Fourier transform of this measure, viewed as a positive definite measure. A set will be called *pure point diffractive* if this Fourier transform is itself a pure point measure, where the spectrum may be a dense set of points.

A special case of this notion of diffractivity is given by the *Poisson summation formula* (PSF). Given a lattice $\varGamma \subset \mathbb{R}^d$, consider the locally finite measure (Dirac comb) $\delta_{\varGamma} := \sum_{x\in\varGamma} \delta_x$, where δ_x is the normalised Dirac measure at x. In this case, the autocorrelation measure of $\delta_{\varGamma}$ is a scaled multiple of $\delta_{\varGamma}$. Its Fourier transform[2] is a (different) scaled multiple of $\delta_{\varGamma^*}$, where $\varGamma^*$ is the dual lattice of $\varGamma$ A generalisation of this formula shows that

[2]The PSF is more commonly written as the evaluation of a function against this tempered distribution $\delta_{\varGamma}$, in which one side of the formula is the sum $\sum_{x\in\varGamma} f(x)$ and the other side is a weighted sum of the Fourier transform of f evaluated on the dual lattice.

an ideal crystal is pure point diffractive, with its spectrum supported on a Delone set, the dual lattice Γ^*.

The cut and project construction leads to many Meyer sets with pure point diffraction spectrum. In particular, regular model sets have this property. A formula for the diffraction of cut and project sets was independently found by many people, including Elser (1986). A mathematically rigorous approach was developed later, starting with work by de Bruijn (1986), Hof (1995) and Schlottmann (2000). The Delone set condition on the initial set can be relaxed, as demonstrated for the visible lattice points in $\mathbb{R}^d$ by Baake, Moody and Pleasants (2000). This set is pure point diffractive, but not relatively dense.

My survey [7] from 2000 discussed results on diffractivity and their relation to classes of almost periodic functions. That paper formulated questions concerning the existence of pure point measures supported on Delone sets having pure point diffraction measures with uniformly discrete or Delone set support. This research area is active and has had substantial recent advances. In 2015, Lev and Olevskii [9] showed that, in the one-dimensional case, all such measures come from the Poisson summation formula. For higher dimensions, there are many exotic examples, found by Favorov, Lev and Olevskii, Meyer, and Kolountzakis; see [13] and references therein. Further advances in both directions are made in [10].

The diffraction spectrum of various aperiodic sets which possess an inflation factor has been much studied. Some of these sets have pure point spectrum, in other cases they have mixed spectrum. It is an open problem whether such inflation sets, when their autocorrelation is a pure point measure, must necessarily have an inflation factor that is a PV number. In another direction, the diffraction spectrum of a Delone set can be related to to the dynamical spectrum of an associated dynamical system with a translation action by $\mathbb{R}^d$ (or, in the lattice-periodic setting, by $\mathbb{Z}^d$); see [1] for a survey.

A famous inverse problem for X-ray diffraction is that of reconstructing the atomic structure of a periodic crystal from X-ray diffraction data. This problem requires overcoming the difficulty that diffraction data determine the intensities of spots but lose the phase information.[3] Consequently, the diffraction image cannot tell certain periodic structures apart. Such structures are called *homometric* and were studied by Pauling and Patterson in the 1930/40s. A Nobel Prize in Chemistry was awarded in 1985 to Hauptmann and Karle 'for outstanding achievements in the development of direct

[3]In terms of Fourier transforms, the scattering intensities record the squared absolute values of the Fourier amplitudes (or coefficients).

methods in the determination of crystal structure' to recover phase information. It is an open problem to determine suitable 'phase information' that might be associated with a diffractive aperiodic set; see [8] for first steps towards a classification. In this context, it is also important to investigate how modulated structures can be distinguished. These questions suggest the investigation of new classes of almost periodic functions.

Connections with number theory

There is an unreasonably effective connection of quasicrystalline structures with algebraic number theory, which already appears in the title of Meyer's 1972 book [11] in which he introduced the notion of what one now calls model sets (simply called 'model' there).

Classical problems in number theory produce crystalline structures with extra symmetries given by Galois group actions. Consider the ring of integers $\mathcal{O}_K$ of an algebraic number field K for which K is a Galois extension of the rational numbers $\mathbb{Q}$ with (finite) Galois group G. Such a ring of integers possesses a Minkowski embedding, compare [AO1, Sec. 3.4], as a lattice in a suitable Euclidean space $\mathbb{R}^d$ (of dimension $d = [K : \mathbb{Q}]$), in such a way that the symmetries of the Galois group G act linearly on the coordinates of this Euclidean space, and leave the lattice $\mathcal{O}_K$ invariant. For example, take G to be the alternating group A_5 of order 60, which is the rotation symmetry group of the regular icosahedron and the smallest non-Abelian simple group. One can find an irreducible equation of degree 5 over $\mathbb{Q}$ whose splitting field (normal Galois closure) has group A_5. The ring of integers of the normal closure of this field then carries an action of A_5, and the restriction to a suitable sublattice can give an (inefficient) cut and project construction.

This lattice embedding of algebraic integers was used by Minkowski in his 'Geometry of Numbers'. His study of lattice packings of convex bodies was invented, in part, to prove results in number theory related to bounds for discriminants of number fields and finiteness of class numbers of algebraic number fields.

The Poisson summation formula plays an important role in number theory, connecting it to harmonic analysis. The functional equation of the Riemann zeta function encodes the PSF in one dimension, and vice versa. The property of pure point diffractivity for certain lattice Dirac combs is another instantiation of the PSF. The existence of quasicrystals which appear to have pure point diffraction spectrum hints at the existence of new kinds of summation formulas generalising the PSF, a problem raised by Dyson [4], who asked whether it might shed light on the Riemann hypothesis. The 'explicit formulas' of prime number theory have a form resembling the PSF, preserving discreteness of point sets but not preserving the Delone set property.

Many of the topics above have been introduced and discussed in [AO1]. The present volume presents chapters surveying and extending several of these topics. The first chapter studies inflation tilings, and the second chapter considers the problem of reconstructing the parameters of model sets from tomographic data. The subsequent chapter considers enumeration problems for embedded sublattices which are related to crystallographic questions. Three further chapters present a detailed account of the structure of almost periodic measures, in a form useful for advancing the study of diffractivity of aperiodic structures. The volume concludes with an epilogue on the physical precursors to the discovery of quasicrystals.

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Preface

This is the second volume in a series of books exploring the mathematics of aperiodic order. While the first volume was meant as a general introduction to the field, we now start to develop the theory in more depth. To do justice to the rapidly expanding field, we decided to work with various authors or teams of authors, which means that this book is somewhere intermediate between a monograph and a review selection. Future volumes will also be structured in this way.

Clearly, almost periodicity is a central concept of crystallography, as it reflects and captures the coherent repetition of local motifs or patterns. The foremost tool to analyse such structures is provided by Fourier analysis of measures, which thus forms a substantial part of this volume. Other important aspects are usually analysed by group theoretic or general algebraic methods. In this respect, due to the availability of comprehensive reviews and several books, we decided to not include a chapter on space groups and their generalisation to quasicrystals.

The main text begins with a chapter on inflation tilings, contributed by Dirk Frettlöh. It augments the discussion of the first volume by presenting a panorama of less familiar constructions and recent developments. This is followed by a contribution to the inverse problem of discrete tomography, where special emphasis lies on the comparison between notions from classical (periodic) crystallography and their extensions to quasicrystals. A similar interplay is prevalent in the ensuing chapter on enumeration problems for lattices versus embedded $\mathbb{Z}$-modules, which highlights the power of number-theoretic methods in the theory of aperiodic order.

The substantial part on almost periodicity and its facets begins with a thorough exposition of the general theory of almost periodic measures on locally compact Abelian groups, contributed by Robert V. Moody and Nicolae Strungaru. This comprehensive summary emerged from the need to understand the spectral structure of aperiodic systems. Perhaps the most important connection exists with the structure of Meyer sets and their description via cut and project schemes, which is developed in the ensuing chapter by Nicolae Strungaru. This part is concluded by an expository discussion of

the sampling problem for (almost) periodic functions along exponential sequences, which highlights yet another connection with number theory.

Complementing the foreword by Jeffrey C. Lagarias, this volume ends with an epilogue on the emergence of quasicrystals from the perspective of physical sciences, with a focus on the underlying theoretical ideas. This epilogue was contributed by Peter Kramer who is one of the pioneers and founders of the field on the side of theoretical and mathematical physics.

As mentioned above, this volume consists of solicited reviews and thematic additions. All chapters have been edited or partly redrafted by us to match the style of the series and its general notation as far as possible. We have thus made the first volume in the aperiodic order series the main reference for all chapters, and refer to it frequently. Nevertheless, some deviation and/or additions are inevitable as a consequence of the established conventions in different mathematical disciplines. Some other, more minor changes have also occurred, such as distinguishing between inclusion and proper inclusion of sets. Where appropriate, such modifications are detailed in footnotes. Each chapter has its own bibliography, while the general index covers all chapters and is also meant to reflect connections between the expositions.

Let us give some background on the tiling that is shown on the book cover. It was designed by Franz Gähler, and is locally equivalent (in the sense of mutual local derivability) to his shield tiling. It was originally designed for a competition at the Fields Institute for Research in Mathematical Sciences in Toronto in 1995. In this year, the Fields Institute moved from Waterloo to Toronto, where a fundraising tiling on the wall in the backyard was planned. Gähler's submission won the competition, but, for a number of reasons, the tiling wall was never realised.

Various people have favourably contributed to this volume. First of all, we would like to thank all authors for the effort they have put into the individual chapters, and into critically reading and commenting on other parts of the volume. Furthermore, we are indebted to Franz Gähler, Neil Mañibo, Yasushi Nagai, Dan Rust, Timo Spindeler, Venta Terauds and Christopher Voll for their comments and suggestions, which helped to improve the exposition. Special thanks also to Franz Gähler for providing the cover illustration. Last but not least, we thank the staff from Cambridge University Press for an always smooth cooperation, the German Research Council (DFG) for support through CRC 701, and the School of Physical Sciences at the University of Tasmania in Hobart for its hospitality during several visits, which helped us immensely to complete this volume.

Michael Baake and Uwe Grimm

CHAPTER 1

More Inflation Tilings

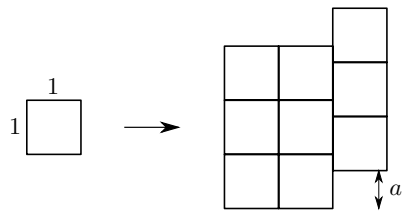
Dirk Frettlöh

Inflation tilings exhibit a wealth of properties, as we shall demonstrate by means of explicit examples. In this sense, this chapter can be seen as an extension of [AO1, Ch. 6]. Along the journey, the concept of inflation will be generalised in several ways. One of the aims of our exposition is to highlight some of the more exotic behaviour that can be observed in the realm of inflation tilings and to point out some interesting questions raised by these examples. Most of the examples discussed below are contained in the Tilings Encyclopedia [21].

1.1. A simple inflation tiling without FLC

Many if not most examples of aperiodic tilings in the literature have *finite local complexity* (FLC); see [11] or [AO1, Sec. 5.3] for background. Even though these examples may be easier to construct, there is no reason to assume that FLC is a typical property of inflation tilings. One of the simplest inflation tilings that fails to have FLC is generated by the following rule [33]:

(1.1.1)



The inflation factor (or multiplier) for this rule is 3, and the single prototile is a unit square. Under the inflation, each square is replaced by three columns of three squares each, where the third column is shifted vertically by some irrational number $a \notin \mathbb{Q}$. The resulting tilings contain pairs of squares sharing an entire edge, as well as pairs of squares sharing part of an edge, where vertical shifts of the form $na \bmod 1$ between adjacent squares are realised with infinitely many different $n \in \mathbb{N}$. In particular, the integer n takes the

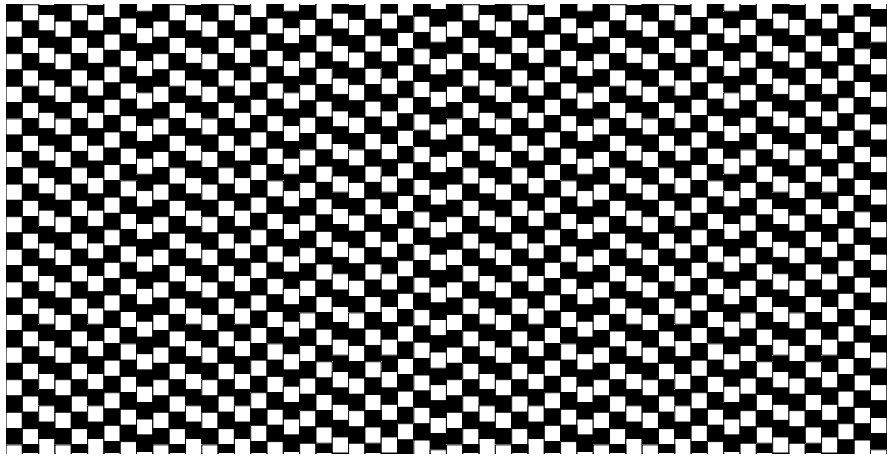
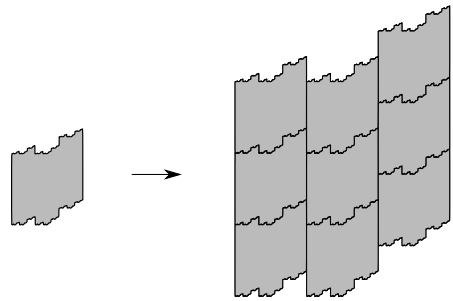


FIGURE 1.1.1. A patch of a simple non-FLC tiling, as defined by Eq. (1.1.1). For clarity, the square tiles are alternatingly coloured black and white.

values 1, $3+1$, 3^2+3+1 etc. Since a is irrational, the corresponding values of na mod 1 are all different. Consequently, there are infinitely many pairwise non-congruent clusters (or patches) of two adjacent tiles. This shows that the tilings obtained from this inflation rule do not have the FLC property. A patch of such a tiling is shown in Figure 1.1.1.

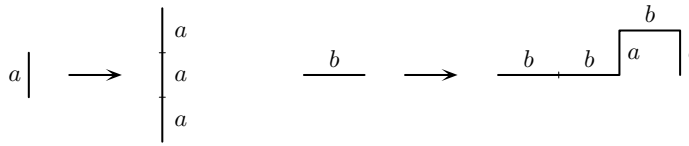
If one does not insist that the tiles are polygons, one can turn the inflation rule (1.1.1) into a *stone inflation* [AO1, p. 148]. Parts of the boundary of the prototile will then be turned into fractals. The corresponding stone inflation is given by



and is clearly mutually locally derivable (MLD) with the inflation (1.1.1); see [AO1, Sec. 5.2] for background on MLD as an equivalence relation.

The boundary of the prototile is not a 'proper' fractal, in the sense that its Hausdorff dimension is 1. This can be seen by employing the methods described in [47]. Denote the upper part of the boundary of the prototile by

F. The stone inflation induces a substitution σ for F, namely



where b denotes a horizontal line segment of unit length and a denotes a vertical line segment of length a. The matrix of this induced substitution is $M = \left(\begin{smallmatrix} 3 & 2 \\ 0 & 3 \end{smallmatrix}\right)$. The contraction factor of the iterated function system (IFS, compare [AO1, Sec. 7.1]) for F is $c = \frac{1}{3}$, the Perron–Frobenius (PF) eigenvalue of M is 3. Loosely speaking, the 'growth rate' of the iterates of the IFS is $3 \cdot \frac{1}{3} = 1$. In order to get a set with dimension strictly larger than 1, the growth rate needs to be > 1. For instance, the growth rate of the Koch curve is $\frac{4}{3}$, which results in its Hausdorff dimension being $\frac{\log(4)}{\log(3)}$.

More precisely, the curve F is only a subset of the solution S of the IFS corresponding to σ, because the IFS has overlaps, and these overlaps yield additional parts of S that are not part of the boundary of the prototile of the tiling. Nevertheless, F is a subset of S, hence its dimension is equal to or less than the dimension of S. Because F has at least dimension 1, it suffices to show that the Hausdorff dimension of S is 1, too. By [47, Prop. 6.106], the *affinity dimension* of S is

$$\dim_{\mathsf{aff}}(S) = \frac{\log(\rho(M))}{\log(c^{-1})} = \frac{\log(3)}{\log(3)} = 1.$$

Here, $\rho(M)$ denotes the spectral radius of M. Due to [47, Prop. 4.122], the Hausdorff dimension of S is bounded by the affinity dimension, hence it also equals 1. Consequently, the boundary curve F of the prototile has Hausdorff dimension 1 as well.

There are more sophisticated but essentially similar constructions of non-FLC inflation tilings by Danzer [6, 7] as well as by Frank and Robinson [14]; see also [AO1, Ex. 5.8] as well as [12]. All of these have in common that they contain infinitely many non-congruent pairs of tiles along a 'fault line' in the tiling. Informally, a fault line is an infinite line that separates a tiling into two halves, such that sliding the half tilings along the fault line produces tilings that still belong to the same hull. More precisely, in any given inflation tiling with an infinite fault line, there occur (countably) infinitely many distinct ways that two tiles are shifted against each other along the fault line. These shifts form a set that will have limit points. The tiling orbit closure in the local topology will then also contain tilings with shifts that correspond to these limit points, which might possibly be arbitrary real numbers.

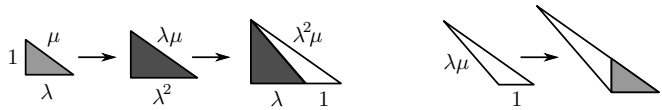
Fault lines are a typical phenomenon of non-FLC tilings. In fact, it is shown in [14] (in the proof of Thm. 4.4) that primitive stone inflations either produce FLC tilings or tilings with a fault line. Some non-trivial sufficient conditions for inflation tilings to have FLC are given in [16] and [14].

1.2. One-parameter families of inflation rules

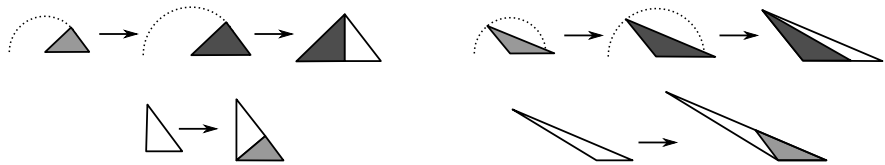
Usually, inflation rules are rigid in the sense that one cannot continuously deform the tiles without destroying the inflation property. Here, we discuss a different example of an inflation rule due to Danzer. It contains one continuous parameter which determines the shapes of the tiles. It can be found in the extended version of a paper by Goodman-Strauss [28], which is available from his website.[1]

We consider the following inflation rule for three triangular prototiles

(1.2.1)



where μ is a free parameter. Figure 1.2.1 shows a patch of a tiling arising from this inflation rule. The inflation factor $\lambda \approx 1.3247$ is the largest root of the polynomial $x^3 - x - 1$. It is the smallest Pisot–Vijayaraghavan (PV) number, sometimes called the 'plastic' number; compare [AO1, Ex. 2.17]. The value of μ can be chosen arbitrarily from the open interval $(\lambda-1, \lambda+1)$. Equivalently, the interior angle in the lower left vertex of the small triangle (leftmost in the inflation rule (1.2.1)) can be chosen arbitrarily from the interval $(0, \pi)$. In particular, we can produce tilings with arbitrarily 'thin' tiles in this way. The inflation rules for two further choices of μ are shown below. On the left, a realisation with three right-angled triangles is shown, while on the right the inflation uses three obtuse triangles.



Continuously decreasing or increasing the value of μ corresponds to moving the upper vertex of the first two prototiles along the half-circles indicated by dashed arcs. The upper vertex of the third prototile then moves on a different conic section. We leave it to the reader to work out the details of the latter (which is an ellipse).

[1] `http://comp.uark.edu/~strauss/`

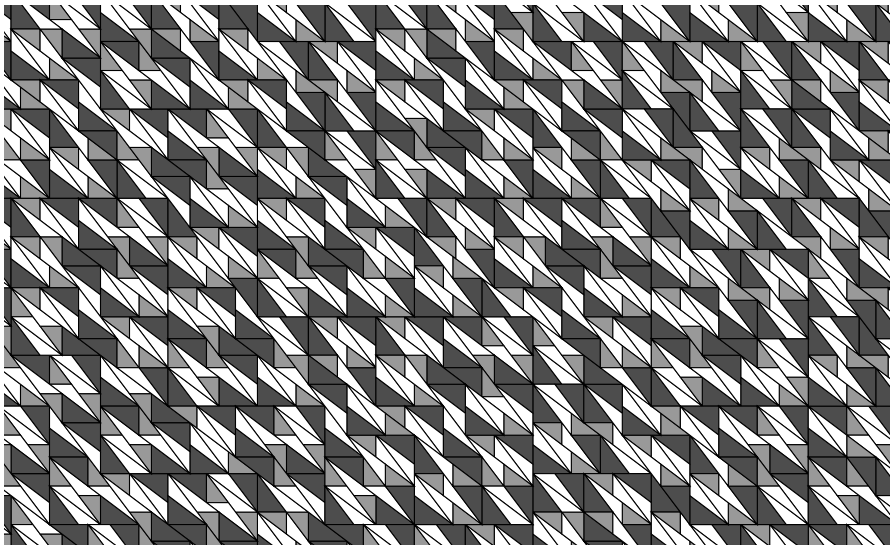
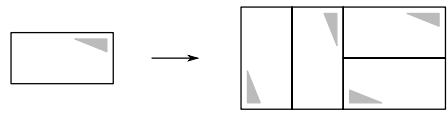


FIGURE 1.2.1. A patch of an inflation tiling generated by the inflation rule (1.2.1). Here, $\mu = \sqrt{\lambda^2 + 1}$, wherefore two of the triangles are right-angled.

1.3. A tiling with non-unique decomposition

A close relative of the table tiling (see [43] or [AO1, Ex. 6.2] for the latter) is the tiling defined by the inflation rule



If one ignores the triangular marks in the diagram, the inflated tile has less symmetry than the prototile. Hence, without the triangular marks, the diagram does *not* define an inflation uniquely. As a consequence, the tiling with unmarked tiles violates local recognisability and thus does *not* possess a *local inflation deflation symmetry* (LIDS) in the sense of [AO1, Def. 5.16]. This is indicated in the right-hand part of Figure 1.3.1.

The tiling with triangular marks does have an LIDS, as it ought to have, according to the following result by Solomyak.

Theorem 1.3.1 ([51, Thm. 1.1])**.** *A self-affine tiling that has FLC with respect to translations has the unique composition property if and only if it is non-periodic.* □

In our terminology, a self-affine tiling is an FLC tiling originating from a primitive stone inflation, and the unique composition property refers to

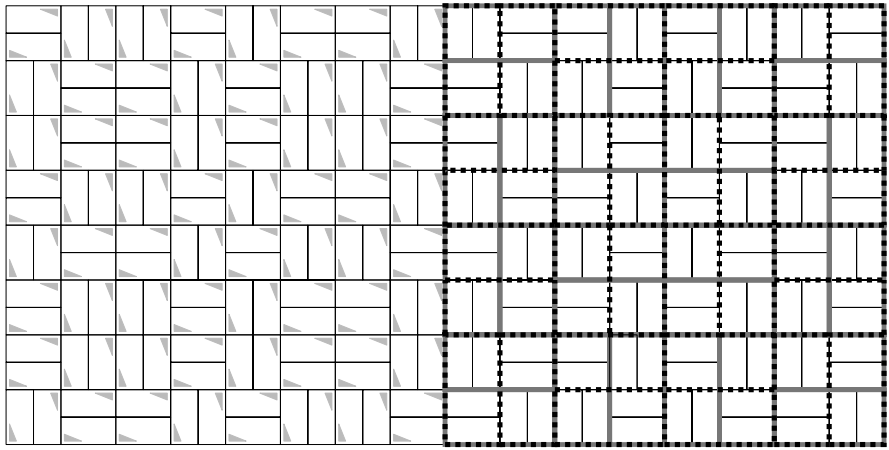


FIGURE 1.3.1. If one ignores the triangular marks in this aperiodic tiling, it has more than one possible preimage under the inflation rule. Two preimages are indicated in the right part of the figure, supertiles of one possibility with grey lines, supertiles of the other with dashed lines.

the LIDS. More precisely, the unique composition property in [51] does not require the supertiles to be determined locally. For the example at hand, this makes no difference. The tilings (marked as well as unmarked) are easily seen to be non-periodic (and hence aperiodic), either by applying Theorem 1.3.1 or by superimposing a hierarchical pattern of squares as in [AO1, Ex. 5.11]; see also [AO1, Fig. 6.50]. This example was discussed by Goodman-Strauss in [27]; see also the extended version of [28] mentioned previously.

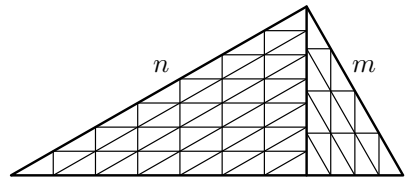
1.4. Überpinwheel

The classical *pinwheel tiling* (see [AO1, Sec. 6.6] and references therein) is an inflation tiling that fails to have FLC with respect to translations, though it has FLC with respect to rigid motions. The tiles in the pinwheel tiling are all congruent (the prototile being a right-angled triangle with edge lengths 1, 2 and $\sqrt{5}$), but they appear in (countably) infinitely many different orientations throughout the tiling. Hence, in order to specify the exact position of some tile in the pinwheel tiling, one needs three parameters with an infinite set of values rather than two; namely, two parameters for the position of its right-angled vertex, say, and one parameter in the circle $\mathbb{S}^1$ for the orientation of the tile. In the sequel, we will often identify the circle with the half-open interval $[0, 2\pi)$. The latter parameter describes the integer multiples of an irrational rotation angle, so is of the form $n\alpha \bmod 2\pi$, where $\alpha = 2\arctan(\frac{1}{2})$.

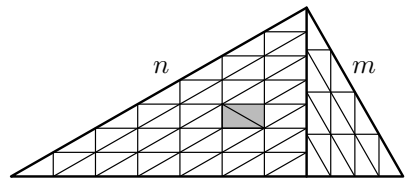
Lorenzo Sadun [45] asked whether there are planar inflation tilings that require two parameters to specify the orientation of the tiles, in the sense that

there are two rationally independent, irrational rotation angles in a tiling. We are now going to discuss an example of such an 'überpinwheel' inflation tiling.

The pinwheel inflation rule is generalised as follows. Let T be a right-angled triangle with edge lengths m, n, $\sqrt{m^2+n^2} =: \lambda$, where $m, n \in \mathbb{N}$ with $m \neq n$. The classical pinwheel tiling corresponds to the case $m = 1$ and $n = 2$ (or $m = 2$ and $n = 1$). There is a canonical partition of λT into congruent copies of T:

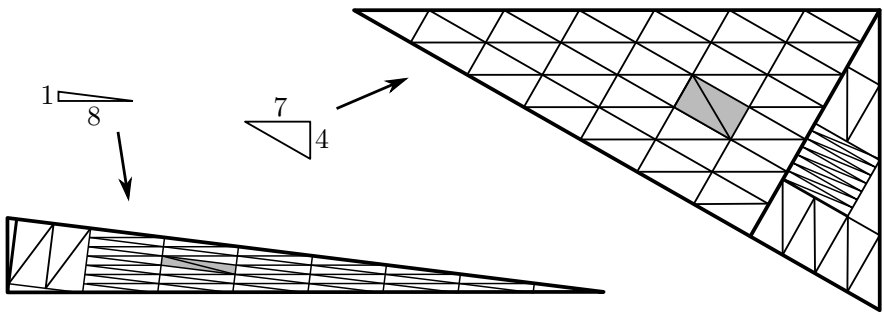


In order to define an inflation rule for an aperiodic tiling with infinitely many orientations, we need to flip at least one (but not all) of the rectangles, for instance as in



Choose an integer N such that $N = \lambda^2 = m^2+n^2 = k^2+\ell^2$ for $k, \ell, m, n \in \mathbb{N}$ with $m \neq n$, $k \neq \ell$ and $\{m, n\} \neq \{k, \ell\}$. Let us take the smallest choice, which is $N = 65 = 1^2 + 8^2 = 4^2 + 7^2$. Let T_1 be a right-angled triangle with edge lengths $1, 8, \sqrt{65}$ and let T_2 be a right-angled triangle with edge lengths $4, 7, \sqrt{65}$.

Consider the pinwheel-like inflation described above, applied to both triangles T_1 and T_2, but in a 'coupled' way. In order to combine these two inflations, replace a rectangular patch of size 7×8 in $\sigma(T_1)$ by a 7×8 rectangular patch of copies of T_2, and vice versa. One possible way to do so is the following:



The next result shows that each tile in the resulting tilings needs two parameters to specify its orientation.

Theorem 1.4.1. *The angles* $\arctan(\frac{1}{8})$ *and* $\arctan(\frac{4}{7})$ *are both irrational, and are independent over* $\mathbb{Q}$.

PROOF. The irrationality of $\arctan(\frac{1}{8}) = \frac{\pi}{2} - \arccos\bigl(\frac{1}{\sqrt{65}}\bigr)$ follows from the fact that $\arccos\bigl(\frac{1}{\sqrt{n}}\bigr) \notin \pi\mathbb{Q}$ for $n \geqslant 3$ odd; see for instance [1, Thm. 3]. This can be proved alternatively using cyclotomic fields. We will illustrate this with $\arctan(\frac{4}{7})$.

If $\arctan(\frac{4}{7}) \in \pi\mathbb{Q}$, then there is an $n \in \mathbb{N}$ such that $(7+4\mathrm{i})^n \in \mathbb{R}$, or equivalently there is an $n \in \mathbb{N}$ such that $\frac{7+4\mathrm{i}}{|7+4\mathrm{i}|}$ is a (complex) n-th root of unity. Then, $\frac{(7+4\mathrm{i})^2}{|7+4\mathrm{i}|^2} = \frac{7+4\mathrm{i}}{7-4\mathrm{i}}$ is also a root of unity. Since $\frac{7+4\mathrm{i}}{7-4\mathrm{i}} \in \mathbb{Q}(\mathrm{i})$, and the roots of unity in $\mathbb{Q}(\mathrm{i})$ are $\{1, \mathrm{i}, -1, -\mathrm{i}\}$ [AO1, Sec. 2.5.2], this yields a contradiction. (More generally, all roots of unity in $\mathbb{Q}(\mathrm{e}^{2\pi\mathrm{i}/n})$ are of the form $\pm\mathrm{e}^{2\pi\mathrm{i}/n}$; see [55, Exc. 2.3] or [AO1, Sec. 2.5.2].)

The independence of $\arctan(\frac{1}{8})$ and $\arctan(\frac{4}{7})$ can again be shown by interpreting them as complex numbers. If $\arctan(\frac{1}{8})$ and $\arctan(\frac{4}{7})$ were dependent over $\mathbb{Q}$, then there would exist $k, m \in \mathbb{Z} \setminus \{0\}$ such that $k\arctan(\frac{1}{8}) = m\arctan(\frac{4}{7})$. With $z := \frac{8+\mathrm{i}}{|8+\mathrm{i}|}$ and $y := \frac{7+4\mathrm{i}}{|7+4\mathrm{i}|}$, this implies that $z^k = y^m$, hence $z^{2k} = y^{2m}$, which gives

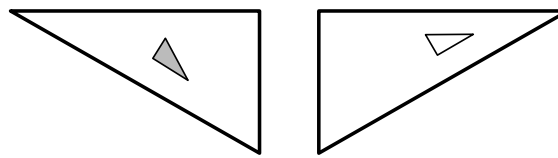
$$\frac{(8+\mathrm{i})^k}{(8-\mathrm{i})^k} = \frac{(7+4\mathrm{i})^m}{(7-4\mathrm{i})^m} \quad \text{and thus} \quad (8+\mathrm{i})^k(7-4\mathrm{i})^m = (8-\mathrm{i})^k(7+4\mathrm{i})^m.$$

Because the ring $\mathbb{Z}[\mathrm{i}]$ of Gaussian integers is a unique factorisation domain, the prime factorisation is unique up to units in $\mathbb{Z}[\mathrm{i}]$, hence

$$(-\mathrm{i})^k(1{+}2\mathrm{i})^k(3{+}2\mathrm{i})^k(1{-}2\mathrm{i})^m(3{+}2\mathrm{i})^m = \mathrm{i}^k(1{-}2\mathrm{i})^k(3{-}2\mathrm{i})^k(1{+}2\mathrm{i})^m(3{-}2\mathrm{i})^m$$

and thus $(1{+}2\mathrm{i})^{k-m}(3{+}2\mathrm{i})^{k+m} = (1{-}2\mathrm{i})^{k-m}(3{-}2\mathrm{i})^{k+m}$. Since $1{+}2\mathrm{i}$, $1{-}2\mathrm{i}$, $3+2\mathrm{i}$ and $3-2\mathrm{i}$ are pairwise coprime in $\mathbb{Z}[\mathrm{i}]$, this yields a contradiction. □

The fact that copies of both T_1 and T_2 occur in $\sigma(T_1)$ as well as in $\sigma(T_2)$ implies the primitivity of σ. Furthermore, the fact that $\sigma(T_2)$ contains two copies of T_2 that are reflected in their shortest edge ensures that the tiles in the corresponding tilings appear in infinitely many orientations. Indeed, substituting these two tiles yields two copies of T_2 that are rotated against each other by $2\arctan(\frac{4}{7})$,



Consequently, higher level supertiles contain copies of T_2 that are rotated against each other by an angle of $n \cdot 2\arctan(\frac{4}{7})$ for all $n \in \mathbb{Z}$. Since we have $\arctan(\frac{4}{7}) \notin \pi\mathbb{Q}$, these angles are distinct. In fact, whenever such a situation occurs, the angles are even uniformly distributed in $[0, 2\pi)$ by [19, Prop. 3.4 and Thm. 6.1]. This result is due to Radin [42] for the pinwheel tiling, while the general case is treated in [19].

Theorem 1.4.2 ([19, Prop. 3.4 and Thm. 6.1])**.** *Let σ be a primitive inflation rule in $\mathbb{R}^2$. Each tiling in the hull of σ has statistical circular symmetry if and only if there is a level-n supertile (for some $n \geqslant 1$) containing two copies of the same prototile which are rotated against each other by some angle $\alpha \notin \pi\mathbb{Q}$.* □

Here, statistical circular symmetry means that the orientations of the tiles are not only dense on the circle, but actually uniformly distributed. Since there are countably infinitely many orientations of tiles in the pinwheel tiling, the uniform distribution property refers to frequencies of tiles with an orientation within certain intervals. Uniform distribution then means that, for any two such intervals of the same length, the frequencies of tiles with orientations in these intervals are equal; see [AO1, Sec. 7.1] for a more precise definition.

Via similar constructions, one may obtain examples of tilings in which the orientations of tiles are described by $M > 2$ irrational angles. This can be done by mixing M pinwheel-like inflations with common inflation factor $\lambda = \sqrt{q}$, where q can be expressed as a sum of two distinct squares in M different ways. Nevertheless, illustrating these examples will be inconvenient, due to the inevitably large inflation factors. The next values are given by $325 = 1^2 + 18^2 = 6^2 + 17^2 = 10^2 + 15^2$ for $M = 3$, by $1105 = 24^2 + 23^2 = 31^2 + 12^2 = 32^2 + 9^2 = 33^2 + 4^2$ for $M = 4$, and by $5525 = 55^2 + 50^2 = 62^2 + 41^2 = 70^2 + 25^2 = 71^2 + 22^2 = 73^2 + 14^2 = 74^2 + 7^2$ for $M = 6$; compare entry A052199 in the OEIS [49].

1.5. Tile orientations with distinct frequencies

The classical pinwheel tiling and its relatives discussed above have the slightly surprising property that the tile orientations are uniformly distributed on the circle. A related result holds for tilings that have FLC with respect to translations.

Theorem 1.5.1 ([20, Thm. 2.3])**.** *Let σ be a primitive inflation rule such that the tilings in the hull of σ have FLC. If, for any two congruent tiles S and T, the patch $\sigma(S)$ is congruent to the patch $\sigma(T)$, the frequencies of congruent tiles with different orientations are equal.* □

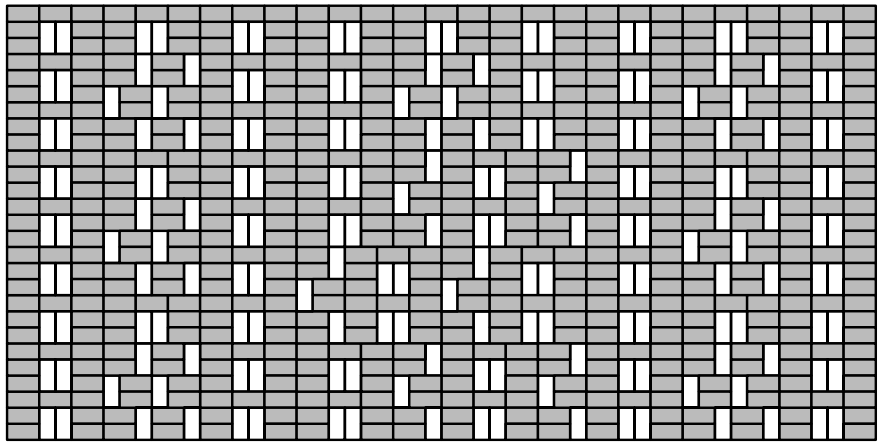
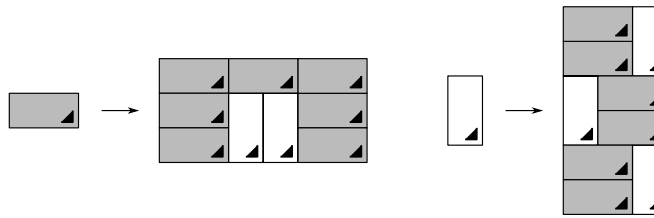


FIGURE 1.5.1. A level-3 inflation patch of the aperiodic 'punch card' tiling (without markers), in which horizontal tiles are more frequent than vertical ones. This requires different inflation rules for horizontal and vertical rectangles, as specified in Eq. (1.5.1).

Note that, throughout [AO1] and thus far in this chapter, we have tacitly taken the compatibility of inflation and rotation for granted. That is, we have implicitly assumed the condition of Theorem 1.5.1 to be satisfied. For instance, if the inflation rule of the Ammann–Beenker tiling is specified by showing the inflation of a square T as $\sigma(T)$, then we implicitly assumed that T rotated by $\pi/2$ is substituted by the patch $\sigma(T)$ rotated by $\pi/2$. However, this need not be the case in general. In order to construct a tiling where, say, horizontal rectangles are more frequent than vertical ones, one needs to specify two different inflation rules for vertical and horizontal rectangles. The following example defines such a rule,

(1.5.1)



We refer to the corresponding tilings as 'punch card' tilings. A patch is shown in Figure 1.5.1. It obviously contains more horizontal rectangles than vertical ones. More precisely, since the inflation matrix is $M_\sigma = \left(\begin{smallmatrix} 7 & 6 \\ 2 & 3 \end{smallmatrix}\right)$ with PF eigenvalue 9 and corresponding right eigenvector $(\frac{3}{4}, \frac{1}{4})^T$, there are three times as many horizontal as vertical rectangles in any tiling of the hull.

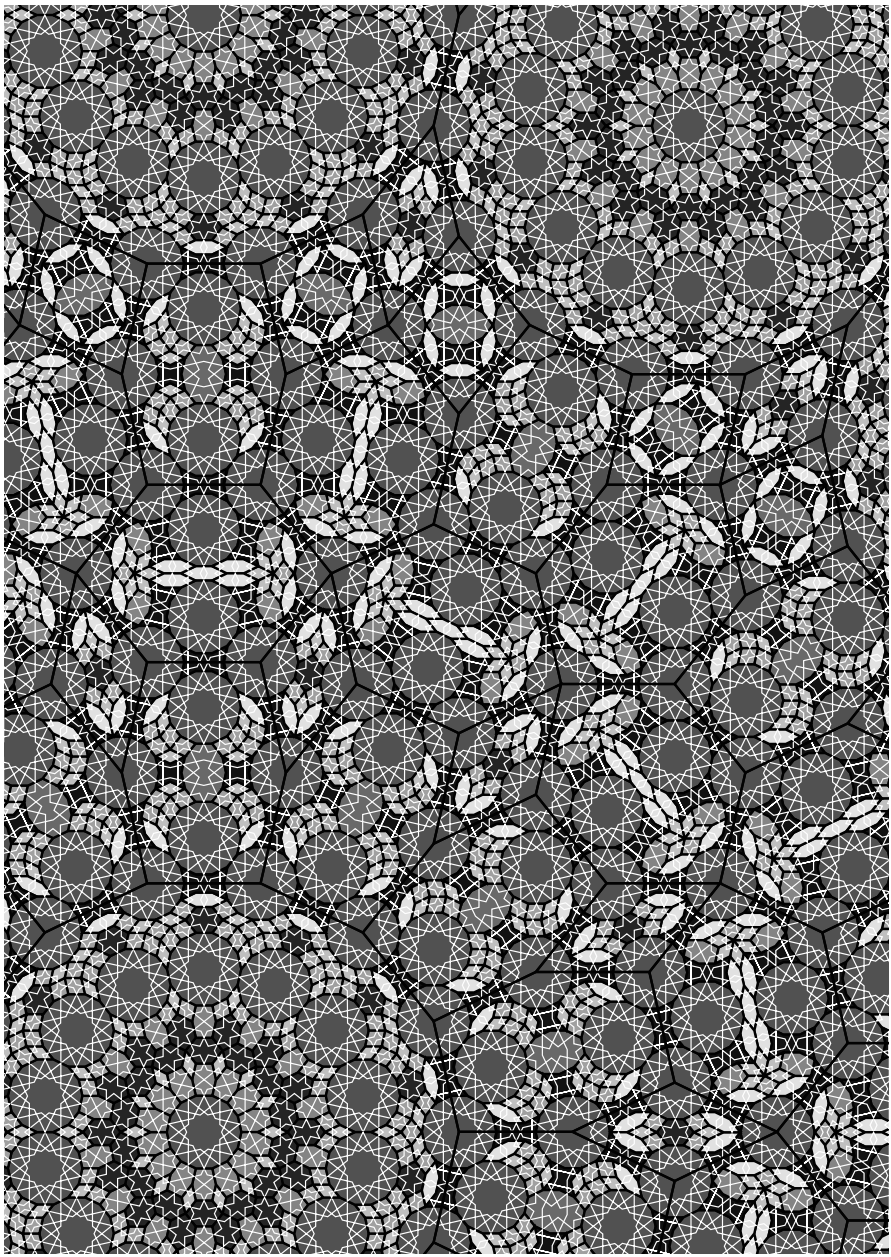


FIGURE 1.6.1. An inflation tiling due to Pautze [40] with 14-fold dihedral symmetry using prototiles inspired by Islamic girih tiles. Level-1 supertiles are indicated by thicker black lines. White lines serve as decoration only.

1.6. Tilings inspired by girih tiles

Many amateur mathematicians have been attracted to inflation tilings, and have devised many new constructions. Some have even substantially influenced the development of the subject, such as, for instance, Robert Ammann [46] and Joan Taylor [50]. The Tilings Encyclopedia [21] further contains examples by Ernesto Amezcua, Laurenz Andritz, Tjipke Hibma, Dale Walton and others; see also the work of Markus Rissanen and Jarkko Kari [32] as well as that of Kurt Hofstetter and the author of this chapter [22].

Several of the constructions are relatively easy to devise, via polyominoes, tangram pieces, or other simple shapes as prototiles. Some of the constructions are considerably more sophisticated. These include inflation tilings inspired by *girih patterns*,[2] which are sophisticated designs in Islamic architecture; see for instance [5] and references therein. While girih patterns usually are not true inflation tilings, the Tilings Encyclopedia [21] contains examples of proper inflation tilings that are based on similar building blocks.

In Figure 1.6.1, we show an example based on 7-fold variants of girih tiles. This inflation tiling is due to Stefan Pautze [40]. Its inflation rule requires the rather large inflation factor $2 + 4\cos(\frac{\pi}{7}) + 2\cos(\frac{2\pi}{7}) \approx 6.851$. For this reason, the image only shows a patch of the tiling where some supertiles (and hence the inflation rule) are indicated by bold lines. In particular, there are eleven prototiles altogether, namely two rhombuses, three convex hexagons, two octagons (one convex and one non-convex), three decagons (two convex and one non-convex) and one regular 14-gon. All but the convex octagon occur in Figure 1.6.1. The level-1 supertiles in the figure are indicated by bold black lines. Only supertiles of the two rhombuses, of two of the hexagons, and of the 14-gon are shown. However, it is not too hard to reconstruct the other supertiles, by taking into account that all supertile edges look the same — they are all bisecting a patch consisting of the sequence (14-gon, non-convex decagon, 14-gon) — and that all supertiles have the same symmetries as the prototiles (in most cases, two orthogonal axes of mirror symmetry).

1.7. Cyclotomic rhombus tilings

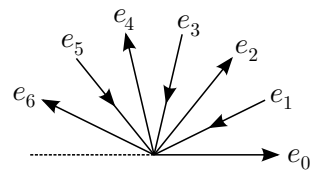
Below, we shall refer to planar aperiodic tilings where all prototiles are rhombuses with interior angles of the form $\frac{k\pi}{n}$ $(n \in \mathbb{N}, 1 \leqslant k \leqslant n-1)$ as *cyclotomic rhombus tilings*. These seem to arise naturally in various contexts, for instance from cyclotomic cut and project schemes; see [AO1, Sec. 7.3]. However, finding simple inflation rules for cyclotomic rhombus tilings can be

[2] Girih is Persian for 'knot'. It refers to decorations in Islamic architecture that are built from interlaced strips, often forming patterns with 6-, 8-, 10- or 12-fold dihedral symmetry.

difficult for larger values of n, such as for $n > 10$, say. In [15], a family of cyclotomic rhombus tilings is obtained by a local derivation from inflation tilings with trapezoids as prototiles. The construction yields cyclotomic rhombus tilings for odd values of $n \geqslant 5$. In [30], Harriss gives inflation rules for cyclotomic rhombus tilings, again for odd $n \geqslant 5$. Recently, Pautze found several constructions that result in cyclotomic rhombus tilings for all $n \geqslant 5$ [40]. It turns out that it is particularly difficult to find consistent inflation rules for the thinnest prototiles (with interior angles $\frac{\pi}{n}$ or $\frac{2\pi}{n}$), where consistency means that no gaps and no overlaps occur when the inflation rule is iterated.

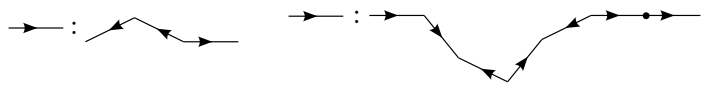
One reason for this difficulty is that there are no interesting stone inflations for rhombuses — dissecting rhombuses into smaller rhombuses only yields trivial dissections, and if all edges have unit length, the inflation factor is always an integer. Hence, one needs inflation rules in which supertiles have protrusions (or bumps) and indentations (or dents); compare the familiar inflation rule for Penrose rhombus tilings; see [11, Fig. 11] or [21]. In a recent paper, Maloney [36] presents a remarkably simple idea which solves this problem for odd values of n. The prototiles are equipped with orientations (indicated by arrows in the figures below). If an edge is parallel to one of the vectors $e_k = \big(\cos(\frac{k\pi}{n}), \sin(\frac{k\pi}{n})\big)^T$ for even k, then it is given the same orientation as e_k, otherwise (for odd k) the opposite orientation. Eq. (1.7.1) shows the situation for $n = 7$,

(1.7.1)



One can then define an edge substitution as follows. An edge in direction e_0 is substituted by a zigzag path of edges in the directions of the e_k. For instance, an edge in direction e_0 can be substituted by an edge sequence $(e_1, -e_6, e_0)$ (left part of Eq. (1.7.2) below), or by $(e_0, -e_5, -e_6, e_2, e_1, e_0, e_0)$ (right part),

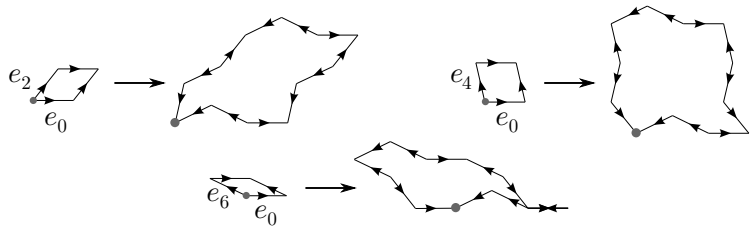
(1.7.2)



Note that, as shown in this example, an edge $-e_k$ points in the opposite direction as e_k, but the direction of the arrow is *not* reversed. For simplicity, one requires that the sequence can be partitioned into pairs $\{-e_k, e_{n-k}\}$ (with $1 \leqslant k \leqslant n-1$), plus an arbitrary number of e_0 directions. This condition implies that the starting point and the endpoint of the sequence lie on the same horizontal line. Rotated edges e_k are substituted by the corresponding

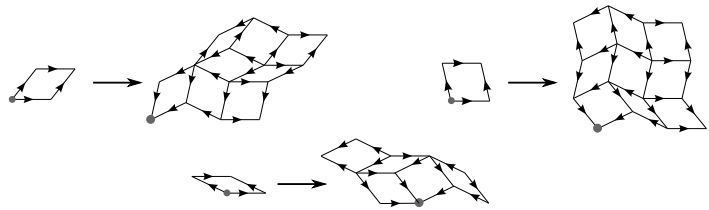
rotated edge sequences. For odd values of k, the orientations of all the arrows are reversed.

This edge rule translates into a skeleton for the inflation of the rhombuses. The four edges of a rhombus with edges in direction e_0 and e_k (with k even) are substituted by the corresponding four edge paths. For instance, for $n = 7$, there are three such rhombuses. Choosing the left edge sequence in Eq. (1.7.2) produces the following partial inflation,



Any edge sequence that yields non-crossing closed edge paths in this manner may be used to define an inflation rule for cyclotomic rhombus tilings. Note that, in the example above, there is one pair of edges that coincide, in the right part of the partial inflation of the bottom tile. In this case, the two edges cancel each other, and will be omitted. By a theorem of Kannan–Soroker [31] and Kenyon [34], the area enclosed by the edge path can be tiled by rhombuses. In general, there are several possibilities to do so. Here, we show one possible way of extending the partial inflation above to an inflation rule:

(1.7.3)



In each step of the construction, one requires that the orientations of edges follow the rule of (1.7.1). Note that the inflation rule diagram above seems to be ambiguous: The prototiles are mirror symmetric, whereas the level-1 supertiles are not. Usually, one breaks the mirror symmetry in the diagram by some markings, as in the example of Section 1.3. This way, the prototiles are given a *chirality*; compare the similar situation for the Lançon–Billard tiling [AO1, Sec. 6.5.1]. Here, the rule is made consistent by the implicit convention that all chiralities in the diagram are the same (that means, reversing the orientation of the arrows corresponds to a rotation of the tile, not to a reflection). As one can check, this implies that tiles of *one* chirality suffice to construct a tiling of the plane, so there is no need to actually draw these additional markings. This chiral inflation rule thus produces a consistent

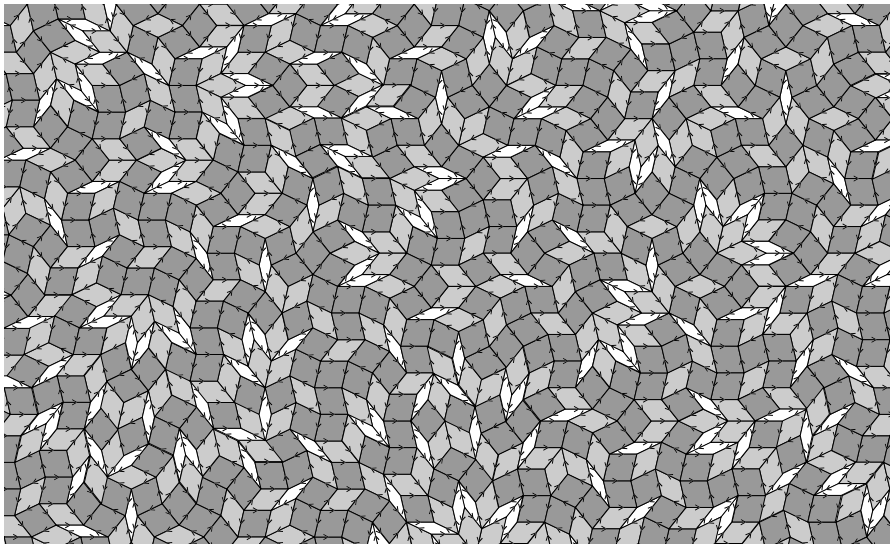


FIGURE 1.7.1. A patch of the cyclotomic rhombus tiling for the inflation rule specified in Eq. (1.7.3).

orientation of the edges in the tilings. Hence, neither gaps nor overlaps will occur for this inflation rule. Figure 1.7.1 shows a patch for this example.

Along similar lines, one aim of [36] was to find inflation rules for cyclotomic rhombus tilings such that not only the hull is invariant under rotation by $\frac{2\pi}{n}$, but that also an individual fixed point tiling is itself invariant. A computer-aided search found an inflation rule of the kind described above for a tiling with 11-fold rotational symmetry. The corresponding edge sequence has length 35, and the inflation factor is approximately 27.2004; see [36] for further details.

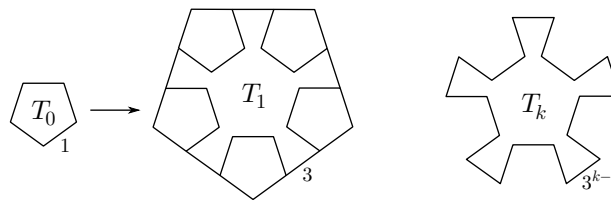
Recently, Kari and Rissanen [32] found inflation rules for cyclotomic rhombus tilings with $2n$-fold rotational symmetry, for arbitrary values of n. Their construction is also based on appropriate edge substitution rules. Here, the edge substitution is made consistent by letting the edges of the supertiles bisect identical sequences of rhombuses which are invariant under rotation by π. In this way, the orientation of edges no longer plays a role. All edge pairs are consistent in the sense that neither gaps nor non-coinciding overlaps occur. The inflation rules are then chosen such that, at the vertices of the supertiles, only tiles with the smallest interior angle $\frac{\pi}{n}$ meet. In the resulting tilings, each supertile vertex is then surrounded by a star that comprises $2n$ rhombuses. This construction yields a fixed point of the inflation with individual $2n$-fold rotational symmetry. For $n = 11$, the inflation factor of this construction is approximately 48.871.

Independently, Pautze described a plethora of inflation rules for cyclotomic triangle tilings and rhombus tilings with n-fold symmetry [40], using smaller (but still generally large) inflation factors.

1.8. Infinitely many prototiles

There are examples of inflation tilings that use finitely many tile shapes up to similarity, but infinitely many prototiles up to congruence. One example emerged in answer to the question of whether there is a tiling of the plane in which all tiles are fivefold symmetric [8]. These tilings are required to be locally finite [AO1, Def. 5.3], and the tiles to be topological disks. It turns out that the answer is affirmative if the tiles are allowed to be arbitrarily large. The following inflation rule provides an example,

(1.8.1)



Here, the prototiles have two distinct shapes. The prototile T_0 is a regular pentagon of unit edge length. The tiles T_k ($k \in \mathbb{N}$) are non-convex, fivefold symmetric 20-gons where all edges have length 3^{k-1}. The inflation $\sigma(T_0)$ is indicated in the figure above, it consists of T_1 and five copies of T_0. For $k \geqslant 1$, let $\sigma(T_k) = T_{k+1} = 3T_k$. This inflation is clearly not primitive: Firstly, no $\sigma^n(T_1)$ contains a copy of T_0, and secondly, there are infinitely many prototiles. Due to the non-primitivity, pathological behaviour may occur. For instance, if we attempt to construct a fixed point tiling by starting from T_1 centred at the origin and applying the inflation, the resulting sequence $T_1, \sigma(T_1), \sigma^2(T_1), \ldots$ converges to 'a single infinite tile'. Nevertheless, the supertiles $\sigma^n(T_0)$ can provide a non-trivial fixed point of σ as follows.

The idea is to find a copy of T_0 in the relative interior of $\sigma^2(T_0)$, hence T_0 can serve as a seed for a fixed point. Consider T_0 to be centred at the origin. Choose a pentagon P (a specific copy of T_0) inside $\frac{1}{9}\sigma^2(T_0)$. Banach's contraction principle applied to this contraction on T_0 yields a fixed point x in the interior of T_0. Now, consider the translate $T_0 - x$. Then,

$$T_0 - x \subset \sigma^2(T_0 - x) \subset \sigma^4(T_0 - x) \subset \sigma^6(T_0 - x) \subset \cdots$$

is a nested sequence that converges in the local topology to a fixed point of the inflation σ. Figure 1.8.1 shows the point x and part of the tiling fixed under the inflation.

Another interesting family of examples with infinitely many prototiles (up to congruence) but finitely many prototiles (up to similarity) is described

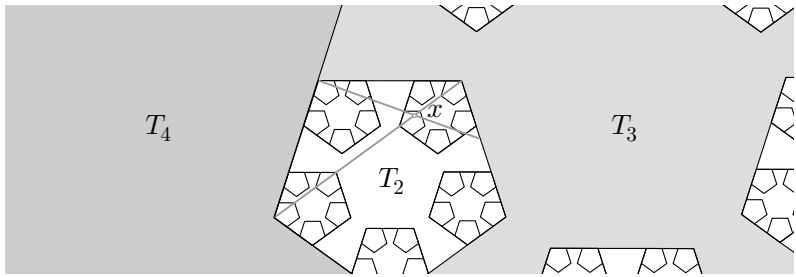
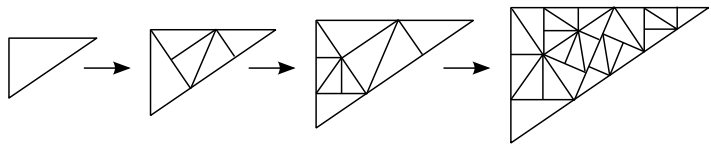


FIGURE 1.8.1. The central patch of a fixed point of the inflation rule (1.8.1) with fivefold tiles. The grey lines indicate how to construct the fixed point x geometrically.

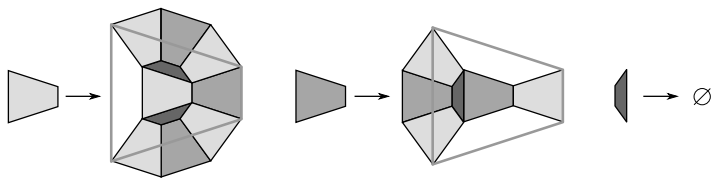
in [44], where Sadun generalises the pinwheel inflation rule to arbitrary right-angled triangles. The rule is that, in each step, the biggest triangles are subdivided topologically according to the pinwheel inflation rule (for the latter, see [AO1, Sec. 6.6]). In the generic case, this construction produces tilings with triangles of infinitely many distinct sizes, which all are similar to each other. The general idea is indicated in the following sketch,



In countably many cases, this construction gives rise to an inflation with finitely many prototiles. In particular, let θ denote the smallest interior angle of the triangle. Then, the inflation rule uses finitely many prototiles if and only if $\frac{\log(\sin(\theta))}{\log(\cos(\theta))} = \frac{p}{q} \in \mathbb{Q}$, with p and q coprime. The number of tile sizes in the tiling is then given by $\max(p, q)$. In the remaining (uncountably many) cases, there are infinitely many prototiles. Even then, the sizes of all prototiles still lie within a certain range [44, Lemma 1], unlike in the fivefold example above, where tiles become arbitrarily large.

1.9. Inflations with an empty supertile

The following inflation rule σ was found by Socolar; see the 'Birds and Bees' entry in the Tilings Encyclopedia [21].

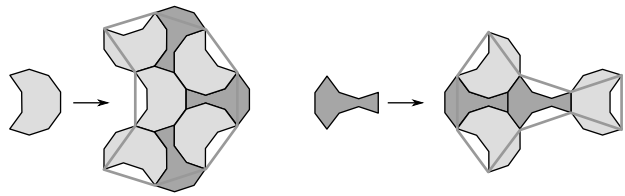


Note that this is not a stone inflation, but still a consistent inflation rule; compare [AO1, Sec. 5.6]. The inflated prototile shape is indicated by the grey lines. This inflation is neither primitive nor even irreducible, because the smallest tile is mapped to the empty set.[3] Thus, the corresponding column of the substitution matrix

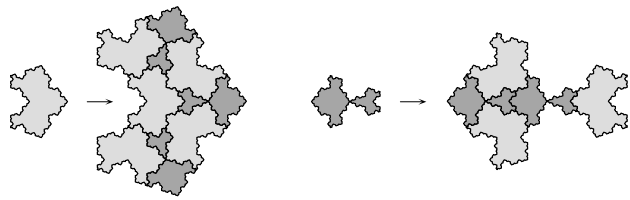
$$M_\sigma = \begin{pmatrix} 5 & 3 & 0 \\ 3 & 2 & 0 \\ 2 & 1 & 0 \end{pmatrix}$$

contains only zeros. Nevertheless, the inflation rule defines a hull which is repetitive and minimal. Since this example is neither primitive nor a stone inflation, the PF eigenvalue of M_σ need not agree with the squared inflation factor. However, here it actually does. The eigenvalues of M_σ are τ^4, τ^{-4} and 0, where $\tau = \frac{1}{2}(1+\sqrt{5}\,)$ is the golden ratio. The prototiles have edge lengths 1 and $\tau^2 = \tau + 1$; the inflation factor is τ^2. So indeed, the PF eigenvalue of the substitution matrix is the squared inflation factor. The right and left PF eigenvectors (up to normalisation) are given by $(\tau^2, \tau, 1)^T$ and $(\tau, 1, 0)$.

In general, although the tile that is replaced by an empty tile may appear superfluous, it may be difficult to find an equivalent inflation (in the sense that it defines a tiling in the same MLD class) for polygonal tiles without including it. In this case, it is easy to see that one can work with the following inflation rule,



Using two prototiles with fractal boundaries, this can be turned into a stone inflation, in the spirit of [AO1, Rem. 6.9]. The resulting inflation rule is



[3] It is instructive to compare this rule with that for Penrose's $(1 + \varepsilon + \varepsilon^2)$-tiling, see [AO1, Ex. 5.13], where one tile is mapped to itself, hence primitivity is also violated. The present example pushes this behaviour even further.

This stone inflation has the symmetric inflation matrix $\left(\begin{smallmatrix} 5 & 3 \\ 3 & 2 \end{smallmatrix}\right)$, with largest eigenvalue τ^4 and corresponding PF eigenvector $(\tau, 1)^T$. This shows that the seemingly meaningless PF eigenvector of the non-primitive matrix above in fact yields the correct inflation factor and correct relative frequencies of the two large prototiles (as well as determining the correct areas of the fractal tiles). Even the vanishing prototile area can be interpreted consistently.

Remark 1.9.1. A close inspection of the 'fractalised' inflation rule reveals that the smaller prototile can consistently be split into two prototiles. This would result in an alternative inflation rule σ' with three prototiles, which produces a tiling in the same MLD class. The corresponding inflation matrix reads

$$M_{\sigma'} = \begin{pmatrix} 5 & 2 & 1 \\ 3 & 2 & 0 \\ 3 & 1 & 1 \end{pmatrix}$$

with PF eigenvalue τ^4 as before, and PF eigenvectors proportional to $(\tau, 1, 1)^T$ (for the frequencies, up to normalisation) and $(3\tau + 1, \tau + 1, 1)$ (for the prototile areas). We leave it to the reader to explore the various connections between these inflations, and to determine the Hausdorff dimension of the prototile boundaries (which follows from their structure as Koch-type curves and is given by $\frac{\log(3)}{2\log(\tau)} \approx 1.1415$). $\Diamond$

Together with the examples of [AO1, Rems. 6.9 and 6.11], this generalised inflation raises two questions. Firstly, it would be interesting to know which proper inflation rules (but possibly with bumps and dents) can be turned, within the same MLD class, into a stone inflation by a change of prototiles, possibly with fractal boundaries. Secondly, one would like to have at least sufficient criteria for when it is possible to replace a generalised inflation rule by a proper one, again under preservation of the MLD class.

1.10. Overlapping tiles

Even though many examples of inflations in [AO1] and in this chapter are actually stone inflations, there are several exceptions, such as the Penrose rhombus tilings [AO1, Sec. 6.2] and the inflation rules for cyclotomic rhombus tilings in Section 1.7. Usually, the non-stone inflations are chosen carefully in such a way that either no overlaps occur at all (bumps of one supertile fill exactly the dents in adjacent supertiles; see for instance the examples in Sections 1.7 and 1.9), or overlapping tiles coincide exactly (such as the Penrose rhombus inflation or Schlottmann's square triangle inflation described in [AO1, Sec. 6.3.1]). In contrast to this, there are rules where the overlaps do not coincide. For instance, the rule in Eq. (1.10.1), which was found by Petra Gummelt [29], allows non-coincident tile overlaps in order to produce tilings

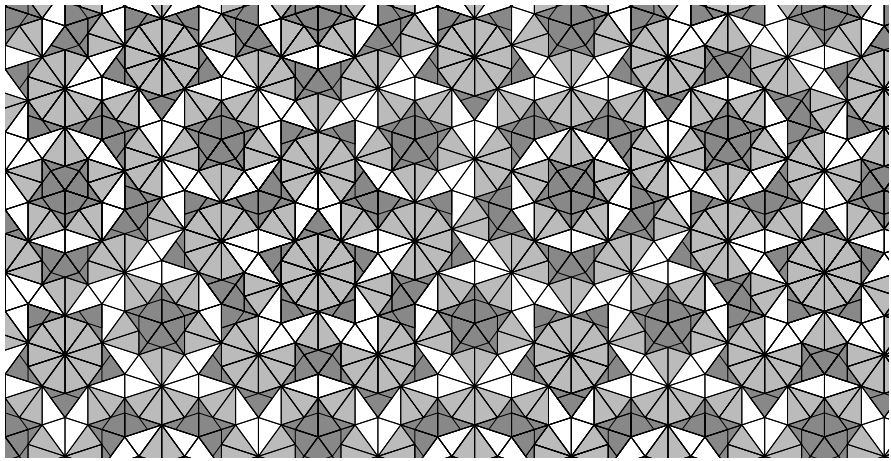
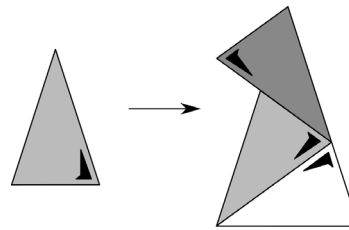


FIGURE 1.10.1. A patch obtained by the overlapping inflation (1.10.1). Note that there is only one kind of overlap, which consists of two dark grey tiles that form a Penrose kite.

with inflation factor $\tau = \frac{1}{2}(1+\sqrt{5})$ with only one prototile (a stone inflation requires at least two prototiles, since the algebraic degree of τ is two).

(1.10.1)



The single prototile T is an isosceles triangle with edge lengths 1, τ and τ. The inflation factor is τ, and $\sigma(T)$ consists of three copies of the prototile, with one of them sticking out. This rule is reminiscent of the Penrose triangle inflation; compare [AO1, Fig. 6.2]. For visual reasons, the three tiles in the image above are distinguished by different shades of grey, but all three are of the same type. Iterating the inflation σ yields several overlaps, where the overlapping tiles do not coincide exactly. Keeping track of all edges, respectively of all partial overlaps of tiles, yields the covering illustrated in Figure 1.10.1. It is straightforward to translate this covering into a tiling, by considering the set of all edges and the partition of the plane they define.

The image is to be understood as showing transparent tiles, so no (parts of) tiles are hidden by other tiles. Obviously, there is only one kind of overlap: Two overlapping dark grey tiles form a 'dart'. This explains the apparent similarity to the Penrose tiling in its kites and darts version. In fact, it is

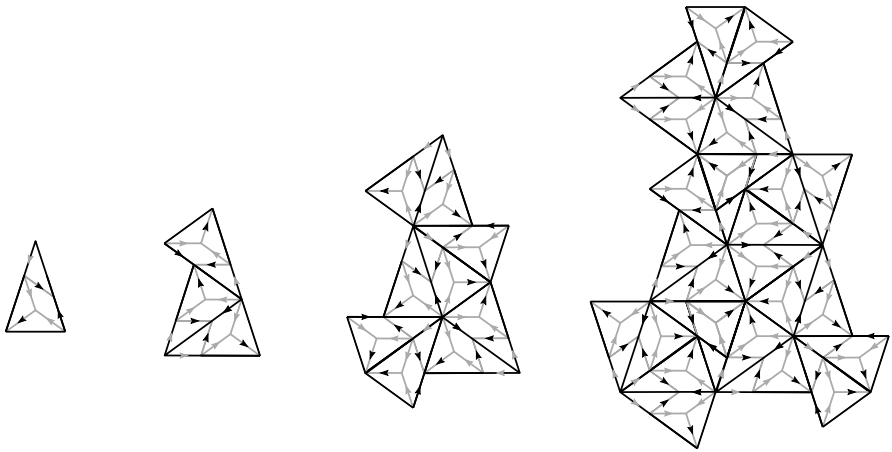
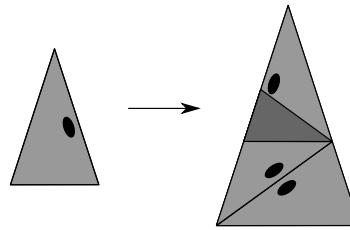


FIGURE 1.10.2. A decoration showing that the overlapping inflation from Eq. (1.10.1) produces tilings that are MLD with Penrose tilings.

not difficult to show that the two versions are MLD, employing the methods described in [AO1, Sec. 6.2]. For instance, via the decoration indicated in Figure 1.10.2, one can establish equivalence with the Penrose rhombus tiling.

Gummelt suggested a similar inflation rule [29] for the golden triangle from above with inflation factor τ, which generates tilings with several different patterns of overlapping tiles,

(1.10.2)



The inflation again uses three copies of a single prototile, but now two tiles overlap in the interior of the level-one supertile. The overlap is indicated by a darker shading in the rule of (1.10.2). It is less clear whether the tilings generated by this rule are MLD to Penrose tilings. A patch of such a tiling is shown in Figure 1.10.3. Similar constructions using overlaps in non-FLC tilings can produce tilings with infinitely many prototiles.

In the examples above, tiles are considered to be *transparent*, hence all edges of overlapping tiles are visible. In contrast to this, there are also tilings with overlaps where some tiles really hide other tiles, or parts of other tiles; and only this overlay structure leads to an aperiodic pattern. The following example illustrates this idea. It is described in [22], where a similar example

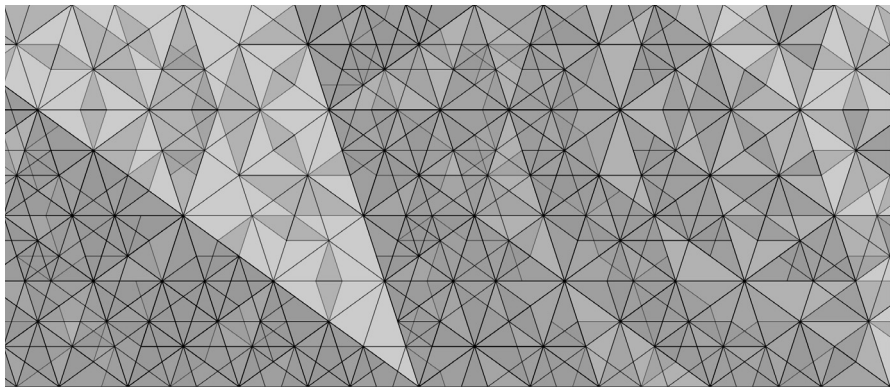


FIGURE 1.10.3. A patch of a tiling generated by the overlapping inflation (1.10.2), with transparent tiles. Darker regions in the tiling correspond to multiple covers in the corresponding covering.

is studied in detail. The construction was found by the artist Kurt Hofstetter, so we refer to such tilings as *Hofstetter tilings*.

The construction proceeds as follows. All tiles are (2×2)-squares. In the first iteration, start from a single square (top of left column in Figure 1.10.4), then place a second square, rotated counterclockwise by $\frac{\pi}{2}$ with respect to the first one, translated by $(1,1)^T$, such that it lies below the first square (second entry in left column). Place a third square, rotated by $\frac{\pi}{2}$ and translated by $(1,-1)^T$ with respect to the second one, below the second square (third entry). A fourth square, rotated by $\frac{\pi}{2}$ and translated by $(-1,-1)^T$

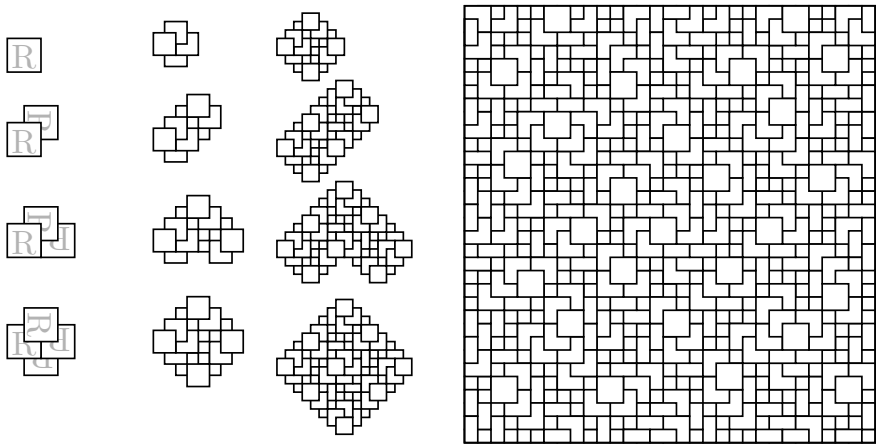


FIGURE 1.10.4. First iterations (four steps each) for generating a Hofstetter tiling (left columns) and a patch of a resulting tiling (right).

with respect to the third square, is placed below the third (and first) square (bottom entry). This constellation of four squares is the building block B_1 for the next generation (second column in Figure 1.10.4). Now repeat the above steps where 'square' is replaced by 'copy of B_1' and the translation vectors $(\pm 1, \pm 1)^T$ by $(\pm 2, \pm 2)^T$ (as shown in the second column). The resulting constellation is denoted B_2. More generally, repeat the same steps for B_i and translation vectors $(\pm 2^i, \pm 2^i)^T$.

The resulting constellations B_n are not patches, but coverings of (part of) the plane. Some of the squares in this covering are covered partially by other squares, a few squares are covered completely. In fact, the covering degree of the resulting coverings is 2 almost everywhere, except close to the boundary of the B_n. In order to translate this into a tiling, we simply omit the covered parts. Since the central part of B_i occurs in the centre of B_{i+1} (for $i \geqslant 3$) the sequence of the B_i converges to a fixed point of the iteration, in the standard local topology.

The examples studied so far [22] are MLD to certain inflation tilings. Nevertheless, similar approaches might yield tilings that are not easily generated by inflations.

1.11. Tiles from automorphisms of the free group

One particular construction of inflation tilings employs automorphisms of the free group F_n with n generators (represented by letters) [54]. Several particular examples have been studied; see for instance [4, 2]. Nevertheless, this method seems less flexible than the inflation method, as most of the inflation tilings described here and in [AO1] cannot be obtained in this way. We describe the general method by using a particular example of Kenyon [35]. This is probably one of the earliest examples of this kind to be found in the literature (but compare the lecture notes [54] for more).

Consider the free group F_3 over 3 letters $\{a, b, c\}$. Let $\Phi \in \mathrm{Aut}(F_3)$ be defined by

$$\Phi(a) = b\,, \quad \Phi(b) = c\,, \quad \Phi(c) = ca^{-1}b^{-2}. \tag{1.11.1}$$

Its image under Abelianisation is the matrix $M_\Phi \in \mathrm{GL}(3, \mathbb{Z})$ given by

$$M_\Phi \;=\; \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & -2 \\ 0 & 1 & 1 \end{pmatrix};$$

see [AO1, Sec. 4.1] for some background. The characteristic polynomial is $p(x) = \det(x\mathbb{1} - M_\Phi) = x^3 - x^2 + 2x + 1$, which is irreducible over $\mathbb{Q}$. Let λ be the (unique) non-real root of p with positive imaginary part. Hence, λ is approximately $0.696 + 1.435\,\mathrm{i}$. This λ acts as our inflation factor. More

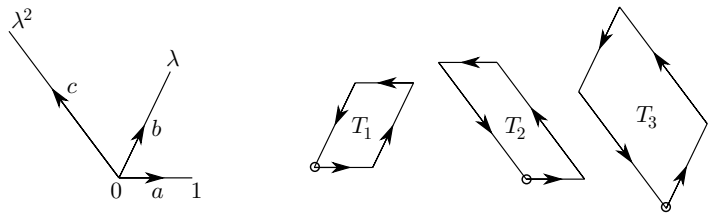
precisely, since it is a (non-real) complex number, it is considered to act in the complex plane, hence it acts as a scaling followed by a rotation. Since $\lambda \cdot 1 = \lambda$, $\lambda \cdot \lambda = \lambda^2$ and $\lambda \cdot \lambda^2 = \lambda^2 - 2\lambda - 1$, which matches the left eigenvector relation

$$(1, \lambda, \lambda^2) M_\Phi \;=\; \lambda\,(1, \lambda, \lambda^2),$$

we may identify a with 1, b with λ, and c with λ^2. More precisely, we consider a, b and c as the *oriented* line segments from 0 to 1, from 0 to λ, and from 0 to λ^2, respectively. Then, the free group commutators

$$aba^{-1}b^{-1}, \quad aca^{-1}c^{-1} \quad \text{and} \quad bcb^{-1}c^{-1}$$

correspond to closed paths. These paths (more precisely, the parallelograms T_1, T_2 and T_3 bounded by them) become our prototiles, where the reference position of each parallelogram is its lower left resp. its lowest vertex point,



The action of Φ on the edges now defines the inflation rule as follows. Since T_1 corresponds to $aba^{-1}b^{-1}$, the relation $\Phi(aba^{-1}b^{-1}) = bcb^{-1}c^{-1}$ means that T_1 is directly mapped to T_3 under the inflation, with preservation of the reference point. For T_2, we get

$$\Phi(aca^{-1}c^{-1}) \;=\; bca^{-1}b^{-1}ac^{-1} \;=\; (bcb^{-1}c^{-1})ca^{-1}(aba^{-1}b^{-1})ac^{-1},$$

which means that T_2 turns into a patch built from one copy each of T_1 and T_3 (the terms in brackets), with specific relative position as given by the term between the brackets. The last factor corresponds to the return to the initial reference point. Likewise, the inflation of T_3 comes from

$$\begin{aligned}\Phi(bcb^{-1}c^{-1}) \;&=\; c^2a^{-1}b^{-2}\;c^{-1}\;b^2ac^{-1}\\ &=\; ca^{-1}(aca^{-1}c^{-1})b^{-1}(bcb^{-1}c^{-1})b^{-1}(bcb^{-1}c^{-1})b^2ac^{-1},\end{aligned}$$

with interpretation analogous to the above. In general, translates of a prototile correspond to conjugates of the word that represents the prototile. This way, the reference point is always reset to its original position. The inflation

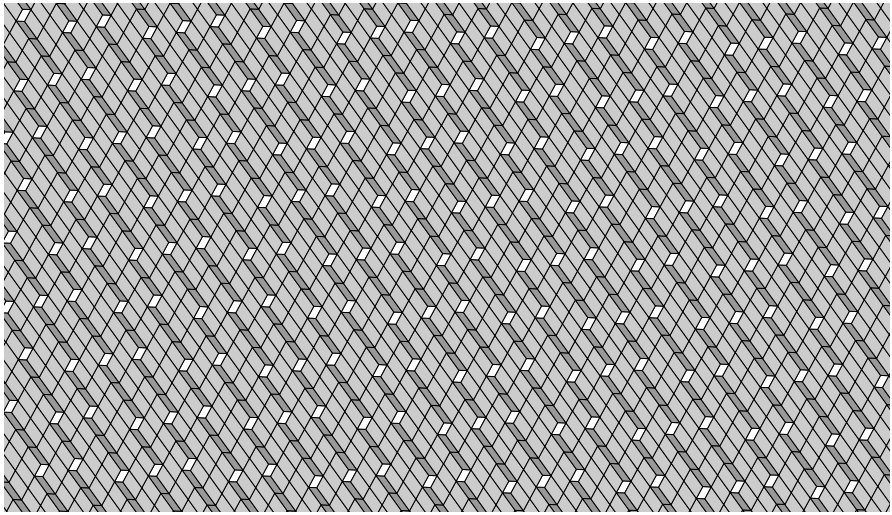
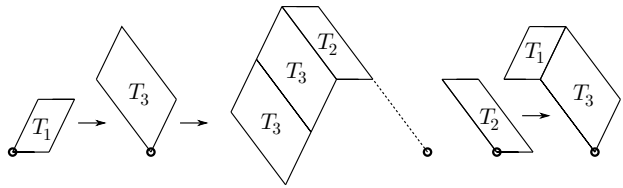


FIGURE 1.11.1. A patch of the inflation tiling with three parallelogram-shaped prototiles, obtained by the rule (1.11.2). The tiling is aperiodic.

for the three prototiles looks as follows,

(1.11.2)



By construction, each tile type appears in only one orientation in the tiling; compare Figure 1.11.1 for an illustration.

Clearly, this inflation is not a stone inflation. By a standard construction, which is based on the original edge inflation (and is similar to the one used in [AO1, Rem. 6.11]), the inflation (1.11.2) can be turned into a stone inflation with fractally shaped (or bounded) prototiles. The shape of the new tiles is illustrated in Figure 1.11.2. The original parallelograms, in the correct relative positions, are indicated for comparison. Note that the new prototiles have 'fractal antennas', which originate from the edge inflation induced by Φ from Eq. (1.11.1). They are the limits of paths that are effectively traversed in both directions. In analogy to the situation of Section 1.7, these antennas can consistently be removed. This corresponds to reducing the edge words as elements within the free group.

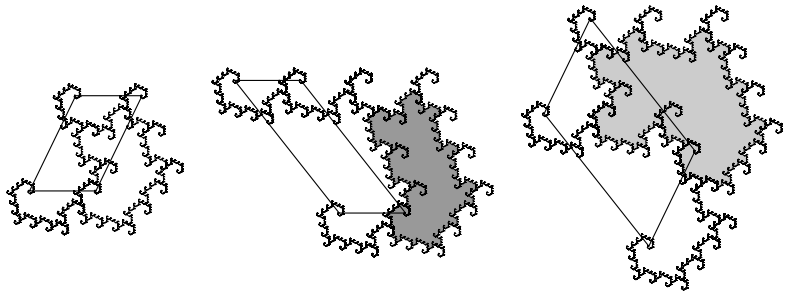
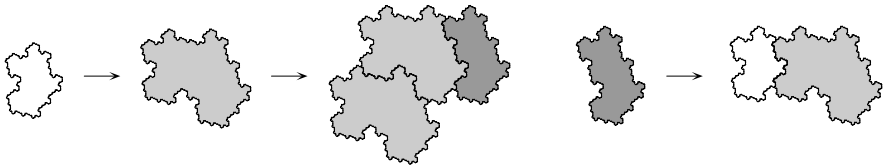


FIGURE 1.11.2. Fractalised versions of the tiles of Eq. (1.11.2).

The induced inflation rule now looks as follows,



where one has to observe that the relative shifts of the fractal tiles with respect to the parallelograms arise as a consequence of the removal of the antennas. This results in a horizontal shift along an edge of type a for T_1 and T_2, while it means a shift along an edge of type b for T_3. The inflation matrix is

$$M = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 2 \end{pmatrix},$$

which also applies to the original inflation rule (1.11.2). The PF eigenvalue is the dominant root of $x^3 - 2x^2 - x - 1$, which is approximately 2.5468. Since it is necessarily real, it is not equal to λ^2, but it equals $|\lambda|^2 = \lambda\overline{\lambda}$. Relative prototile frequencies and areas can be calculated from the right and left PF eigenvectors as usual. Figure 1.11.3 shows a patch of the resulting tiling.

Remark 1.11.1. Due to the complicated path structure of the boundary, which produced the antennas that had to be removed in order to construct the fractally shaped prototiles, the corresponding analysis of the Hausdorff dimensions is considerably more involved than for a simple Koch-type curve. Bernd Sing has analysed this situation [48] and found the following results.

The Hausdorff dimension of the antennas is given by

$$\frac{\log(\kappa)}{\log(|\lambda|)} \approx 1.6355,$$

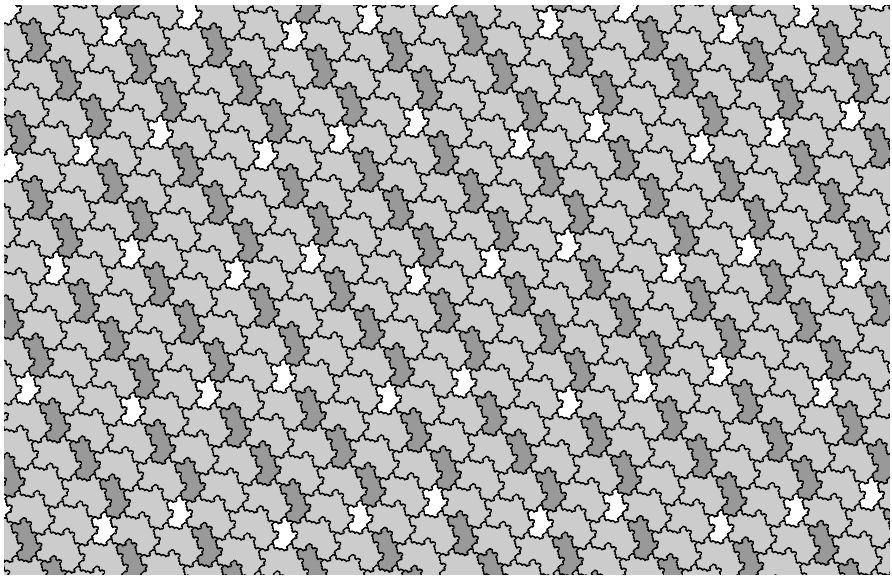


FIGURE 1.11.3. A patch of the fractal version of the inflation tilings.

where $\kappa \approx 2.1479$ is the unique real root of the polynomial $x^3 - x^2 - 2x - 1$. The Hausdorff dimension of the boundaries of the prototiles is considerably smaller. By the standard technique to derive an IFS for the boundary pieces (three are needed here), the Hausdorff dimension turns out to be

$$\frac{\log(\kappa')}{\log(|\lambda|)} \approx 1.1918,$$

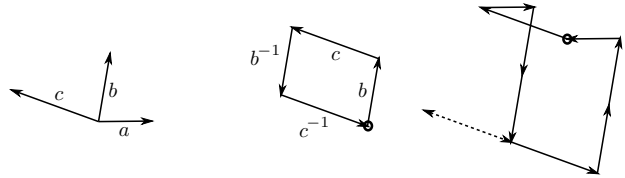
where $\kappa' \approx 1.7455$ is the unique positive real root of the quartic polynomial $x^4 - x^2 - 3x - 1$. ♢

Several other inflation rules can be constructed in this way; browse, for instance, for those entries in [21] that are due to Harriss or Kenyon, or for entries with 'dual' in the title. One may use F_n for $n \geqslant 3$, yielding n line segments and $\binom{n}{2}$ prototiles. In all of these examples, the tiles usually occur in only one orientation in the tiling. Thus, the most prominent inflation rules (such as Penrose, Ammann–Beenker, chair, table and so on) do not arise from automorphisms of F_n in this way. Moreover, not every automorphism of F_n leads to an inflation. On the one hand, the automorphism may not yield an appropriate (complex) value for λ. On the other hand, the polygon given by the edge paths corresponding to $\sigma(T_i)$ is not necessarily tileable by the prototiles. For instance, the edge path might be self-intersecting. As an

example, consider the automorphism

$$\Phi(a) = b\,, \quad \Phi(b) = c\,, \quad \Phi(c) = ab^{-2}c.$$

This yields another complex inflation factor, namely $\lambda \approx 0.215{+}1.307\,\mathrm{i}$. If we identify a with 1, b with λ and c with λ^2 as above, the prototile $bcb^{-1}c^{-1}$ and the edge path $c\,ab^{-2}c\,c^{-1}\,c^{-1}b^2a^{-1}$ of its possible supertile look as follows,



It is not clear whether this technique can produce a proper inflation rule in this case. More generally, it would be nice to derive a criterion to decide which automorphisms of free groups give rise to inflation rules for tilings.

Remark 1.11.2. This construction also has a strong connection to model sets and cut-and-project schemes (CPS, see [AO1, Sec. 7.2]). In general, one may start this construction with an automorphism Φ of the free group with n generators for any $n \geqslant 3$. In the case of $n = 3$, if $\Phi^{-1}(a), \Phi^{-1}(b), \Phi^{-1}(c)$ contain only a, b, c (and not their inverses), the resulting tilings may be generated by a CPS. In particular, if $\Phi(a) = b$ and $\Phi(b) = c$, the PF eigenvector of the inflation matrix M_Φ has entries $(1, \lambda_{\mathsf{PF}}, \lambda_{\mathsf{PF}}^2)$. In this case, a standard construction applies: The fractal version of the two-dimensional tiling generated by Φ as described above is the dual tiling of the one-dimensional tiling generated by Φ^{-1} read backwards; compare [2, 23]. For more on this duality, see [AO1, Rem. 7.6] and references therein, or [17, 18]. ♢

1.12. Mixed inflations

So far, we have encountered several generalisations of inflation rules, such as inflations with infinitely many prototiles or with overlapping tiles, or inflations with empty prototiles. Another generalisation consists of applying not one, but several different inflation rules $\sigma_1, \sigma_2, \ldots, \sigma_n$. These inflations have to be chosen such that they are compatible. For simplicity, they should use the same inflation factor λ and the same prototiles $T_1, \ldots, T_m$. This guarantees that the inflated prototiles λT_i can be dissected according to each of the inflations σ_i. The simplest example one may think of is described in [26]. Consider the two Fibonacci substitutions,

$$\varrho: \begin{array}{l} a \mapsto ab \\ b \mapsto a \end{array} \quad \text{and} \quad \varrho': \begin{array}{l} a \mapsto ba \\ b \mapsto a \end{array};$$

compare [AO1, Ex. 4.6 and Rem. 4.6]. The general idea of mixing these two substitutions can be realised in two different ways.

Firstly, one may apply one out of two substitutions σ_1, σ_2 to *all* tiles in each step: $\sigma_{i_1}(T_1), \sigma_{i_2}(\sigma_{i_1}(T_1))$, etc. If the sequence (i_j) is periodic, this yields nothing new. For example, if the sequence is $122\,122\,122\,122\ldots$, the resulting inflation is just $(\sigma_2)^2\sigma_1$. More generally, we may choose the i_j in a non-periodic manner, either deterministically (according to a Fibonacci sequence, say) or randomly in each step. In doing so, we leave the realm considered so far, and enter the regime of *S-adic* systems; see [41, p. 364]. We refer to [10, 9, 38, 39] for results on ergodicity and complexity of such mixed symbolic substitutions, and to [24] for some results on the cohomology of mixed substitutions.

As far as we know, there are few higher-dimensional examples of this type of construction in the literature; compare [25] and references therein (see also the references in Section 1.13). Note that, in the one-dimensional case, mixing the two Fibonacci substitutions ϱ and ϱ' in this way still generates nothing new, because they both define the same hull. A little later, we shall briefly discuss a two-dimensional example where this type of approach does yield something new.

Secondly, one may apply different substitutions on *individual* tiles randomly. This is briefly described for the two variants of the Fibonacci substitution in [AO1, Sec. 11.2.3]. A random application of ϱ and ϱ' means that one fixes $p \in (0,1)$. Then, in each step of the substitution, a letter b is replaced by a, an a is replaced by ab with probability p, and by ba with probability $1-p$. Such a *random substitution* can conveniently be represented as

$$b \mapsto a \mapsto \begin{cases} ab, & \text{with probability } p, \\ ba, & \text{with probability } 1-p. \end{cases}$$

Considering the resulting sequences as tilings of the real line (with the usual interpretation of a as an interval of length $\tau = \frac{1}{2}(1+\sqrt{5}\,)$ and b as an interval of length 1) one may also ask for diffraction properties of the corresponding tilings. Recent results on the diffraction spectrum were obtained for the hull $\mathbb{X}_{\mathsf{rand}(\varrho,\varrho')}$ of the random Fibonacci substitutions (and more generally, random noble mean substitutions) in [37, 52, 3]. In particular, it is shown that the diffraction spectrum of the random Fibonacci substitution contains no singular continuous part, which was left open in [26].

Theorem 1.12.1 ([37, 52, 3])**.** *The diffraction measure ω of $\mathbb{X}_{\mathsf{rand}(\varrho,\varrho')}$, viewed as a dynamical system, satisfies*

$$\omega \,=\, \omega_{\mathsf{pp}} + \omega_{\mathsf{ac}},$$

where ω_{pp} is a non-trivial pure point measure and where ω_{ac} is a non-trivial

absolutely continuous measure. Simultaneously, this ω is also the diffraction measure of almost all individual elements of the hull. □

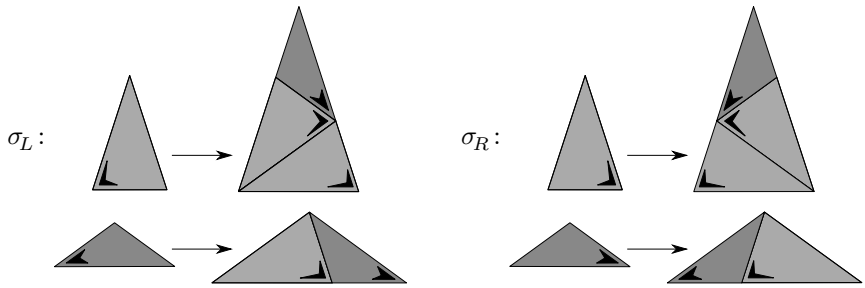
Moreover, exact formulas are given for the intensities of the pure point part of the diffraction spectrum and for the density of the absolutely continuous part. The latter is given in the form of a series that converges uniformly (to the Radon–Nikodym density). The 'almost all' in the theorem above is a consequence of the fact that the usual Fibonacci hull $\mathbb{X}_{\varrho}$ is a (small) subset of $\mathbb{X}_{\mathsf{rand}(\varrho,\varrho')}$. These and other exceptional elements, taken together, have zero measure in the stochastic hull.

Similar results hold for local mixtures of the two possible period doubling substitutions,

$$\begin{aligned} a &\mapsto \begin{cases} ab, & \text{with probability } p, \\ ba, & \text{with probability } 1-p, \end{cases} \\ b &\mapsto aa. \end{aligned}$$

Interestingly, for $p = \frac{1}{2}$, the pure point part of the spectrum vanishes outside $\mathbb{Z}$, whereas it is dense on the real line for $p \neq \frac{1}{2}$; see [3].

Apart from [26], there is very little known about mixed, respectively random, inflations in more than one dimension. A two-dimensional example from [26] uses a chiral variant of the Penrose inflation rule for triangles,



Note that both inflation rules use only rotated and translated copies of the prototiles. Consequently, σ_R is the mirror image of σ_L, and the hulls $\mathbb{X}_{\sigma_L}$ and $\mathbb{X}_{\sigma_R}$ are mirror images of each other (and they are not equal, compare Figure 1.12.1). In contrast to the Fibonacci substitutions ϱ and ϱ' above, σ_L and σ_R define different hulls. Hence mixing them globally (that is, applying one of the two inflations to *all* tiles in each step) yields a much bigger hull $\mathbb{X}_{\mathsf{mix}(\sigma_L,\sigma_R)}$, containing both $\mathbb{X}_{\sigma_L}$ and $\mathbb{X}_{\sigma_R}$. Figure 1.12.2 shows a patch from a tiling in $\mathbb{X}_{\mathsf{mix}(\sigma_L,\sigma_R)}$.

This approach has not yet been studied in detail (but compare Section 1.13). We refer to [25] for more inflations that can be mixed in this way, i.e., inflations with the same factor and the same prototiles. Mixing

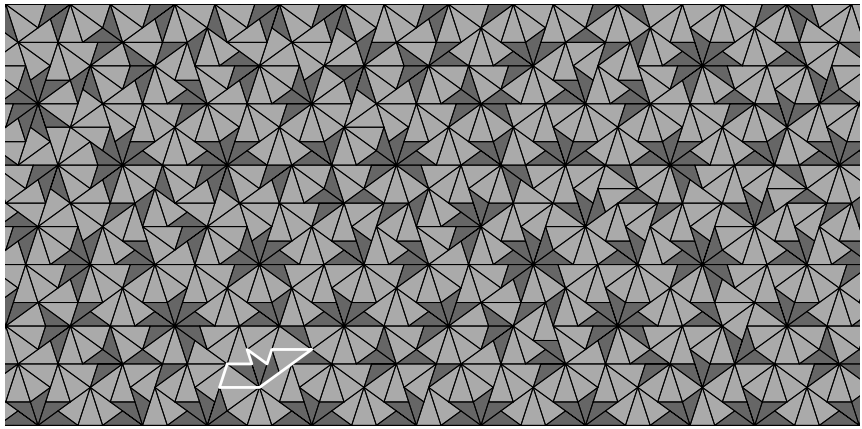


FIGURE 1.12.1. A patch of the left chiral Penrose tiling (in its version with golden triangles) generated by the inflation rule σ_L. Note the small patch consisting of three small triangles and two big triangles in the lower left part, indicated by a white contour. While the tiling contains rotated and translated copies of this patch, it does not contain any reflected copy.

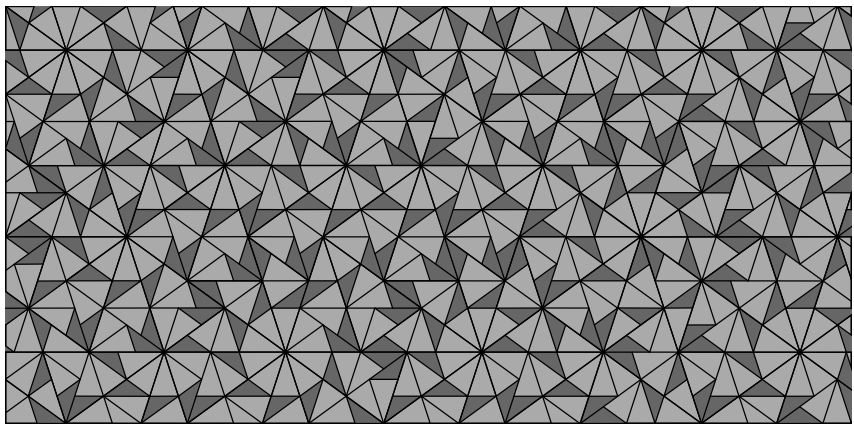


FIGURE 1.12.2. A patch of a mixed chiral Penrose tiling. More precisely, a patch from $(\sigma_2)^2(\sigma_1)^3(\sigma_2)^2(T)$, where T denotes the bigger triangle. Obviously, there are patches in this tiling that do not appear in the chiral Penrose tiling of Figure 1.12.1.

σ_1 and σ_2 locally (that is, applying to each tile σ_1 with probability p, and σ_2 with probability $1-p$) yields an even larger hull $\mathbb{X}_{\mathsf{rand}(\sigma_L,\sigma_R)}$, containing $\mathbb{X}_{\mathsf{mix}(\sigma_L,\sigma_R)}$ (hence $\mathbb{X}_{\sigma_L}$ and $\mathbb{X}_{\sigma_R}$) as subsets. First steps in investigating diffraction properties of the two-dimensional tilings that result from this approach are obtained in [26, 53].

1.13. Fusion tilings

In the previous section, the constructions used different inflations in each step. One may go even further than this. Probably the most general idea goes under the name of *fusion tilings*, which were introduced in [13].

A fusion tiling is generated by the following process. Consider a set of prototiles $\mathcal{P}_0 = \{P_0(1), P_0(2), \ldots, P_0(m_0)\}$. Choose some finite collection of patches, $\mathcal{P}_1 = \{P_1(1), P_1(2), \ldots, P_1(m_1)\}$, where each patch is built from prototiles in $\mathcal{P}_0$. In the next step, choose some finite collection $\mathcal{P}_2 = \{P_2(1), P_2(2), \ldots, P_2(m_2)\}$ of patches that are (measure-wise disjoint) unions of patches in $\mathcal{P}_1$. Continue this process; that is, in step i, choose some finite collection of patches $\mathcal{P}_i = \{P_i(1), P_i(2), \ldots, P_i(m_i)\}$ that are (measure-wise disjoint) unions of patches in $\mathcal{P}_{i-1}$. A tiling $\mathcal{T}$ of $\mathbb{R}^d$ is called a *fusion tiling* (with respect to the family $\{\mathcal{P}_i\}_i$) if any patch in $\mathcal{T}$ is contained in some $P_i(k) \in \mathcal{P}_i$. The family $\{\mathcal{P}_i\}_i$ is called the *fusion rule*.

Note that the tiling space of a fusion rule can be empty, for instance if the inner radii of all patches in the fusion rule are bounded by some common constant. Obviously, all inflation tilings are fusion tilings: Just take the level-n supertiles as the patches in $\mathcal{P}_n$. Moreover, all FLC tilings are fusion tilings: Just define $\mathcal{P}_i$ as the set of all connected patches in $\mathcal{T}$ which contain i tiles or fewer. Consequently, it is plausible that this concept is far too general to prove any reasonable results on fusion tilings. Nevertheless, it is possible to define notions like primitivity or minimality for fusion tilings, and to obtain some general results on fusion tilings that are well-behaved, but still far away from being inflation tilings; see, for instance, [13] for some general results (such as Thms. 4.10, 4.13 and 5.3) and for several amazing examples. This new realm of fusion tilings is much too big to be explored more than superficially in this section.

Let us sketch some possibilities with the following example, which is a variant of [13, Ex. 3.7]. Let the prototiles be two unit squares, distinguished by colour — one black square and one white square, say. The fusion rule is indicated in Figure 1.13.1. It essentially consists of applying different inflation rules in each step. In the language of inflation rules, the level-$(k+1)$ supertile $P_{k+1}(1)$ consists of $2^k \times 2^k$ level-k supertiles $P_k(1)$, surrounded by a collar of $4 \cdot (2^k + 1)$ level-k supertiles $P_k(2)$. The level-$(k+1)$ supertile $P_{k+1}(2)$ is defined analogously, by just reversing the roles of $P_k(1)$ and $P_k(2)$. Hence, the *transition matrices*, which are the matrices counting the number of copies of $P_k(1)$ and of $P_k(2)$ in $P_{k+1}(i)$, are given by $A_k = \begin{pmatrix} 4^k & 4(2^k+1) \\ 4(2^k+1) & 4^k \end{pmatrix}$.

Figure 1.13.2 shows a patch of a resulting tiling. Note that it is generally unclear how to define a fixed point of a fusion rule. However, in this particular example, this is possible. Start with a (2×2)-patch of black squares $P_0(2)$,

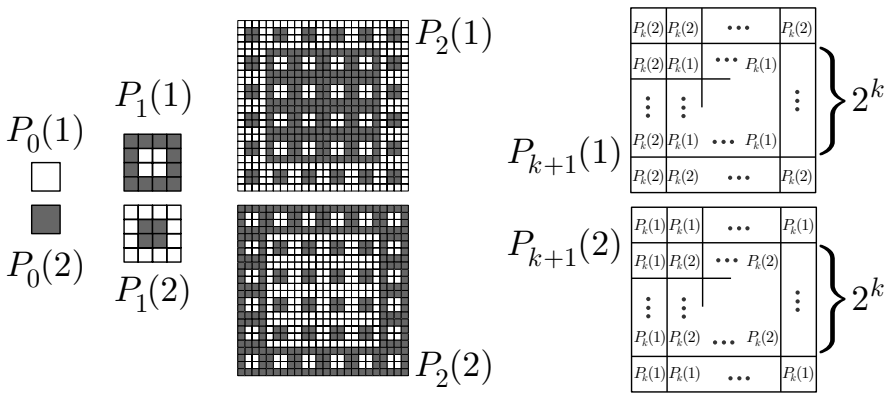


FIGURE 1.13.1. A fusion rule, given by using different inflation rules in each step. In particular, $P_{k+1}(1)$ consists of a $(2^k \times 2^k)$-block of copies of $P_k(1)$ and a collar of copies of $P_k(2)$.

with the common vertex as the origin. The second iteration (four copies of $P_2(2)$ around the origin) contains the first patch in its centre. Inductively, four copies of $P_{2k+2}(2)$ contain a patch of four copies of $P_{2k}(2)$ in its centre. This sequence of patches converges to a tiling $\mathcal{T}$ with respect to the local topology.

This example was chosen for the sake of visualisation. The relative and absolute frequencies of white and black squares are close to $\frac{1}{2}$. More precisely, they are given by the infinite product

$$\frac{1}{2} \pm \frac{1}{2} \prod_{k=1}^{\infty} \frac{2^{2k} - 4(2^k+1)}{2^{2k} + 4(2^k+1)} \;\approx\; \frac{1}{2} \pm 0.002704495,$$

if the seed consists of either black or white squares only, with the larger frequency for the tiles of the same colour as the seed. If one replaces the powers of 2 in the definition of the fusion rule above by powers of 10 (as is the case in [13, Ex. 3.7]), the frequencies become more unbalanced. Firstly, in the analogue $\mathcal{T}'$ of the tiling $\mathcal{T}$ constructed above (starting with four copies of black squares $P_0(2)$), black squares are even more frequent than white squares. Secondly, there is another tiling $\mathcal{T}''$, constructed analogously by starting with four copies of white squares $P_0(1)$, in which white squares are much more frequent than black squares. Here, the frequencies are

$$\frac{1}{2} \pm \frac{1}{2} \prod_{k=1}^{\infty} \frac{10^{2k} - 4(10^k+1)}{10^{2k} + 4(10^k+1)} \;\approx\; \frac{1}{2} \pm 0.177754871.$$

Since both tilings, $\mathcal{T}'$ and $\mathcal{T}''$, contain supertiles of all levels, they are both contained in the hull of $\mathcal{T}'$. Consequently, the hull is not uniquely ergodic, because it supports at least two ergodic measures.

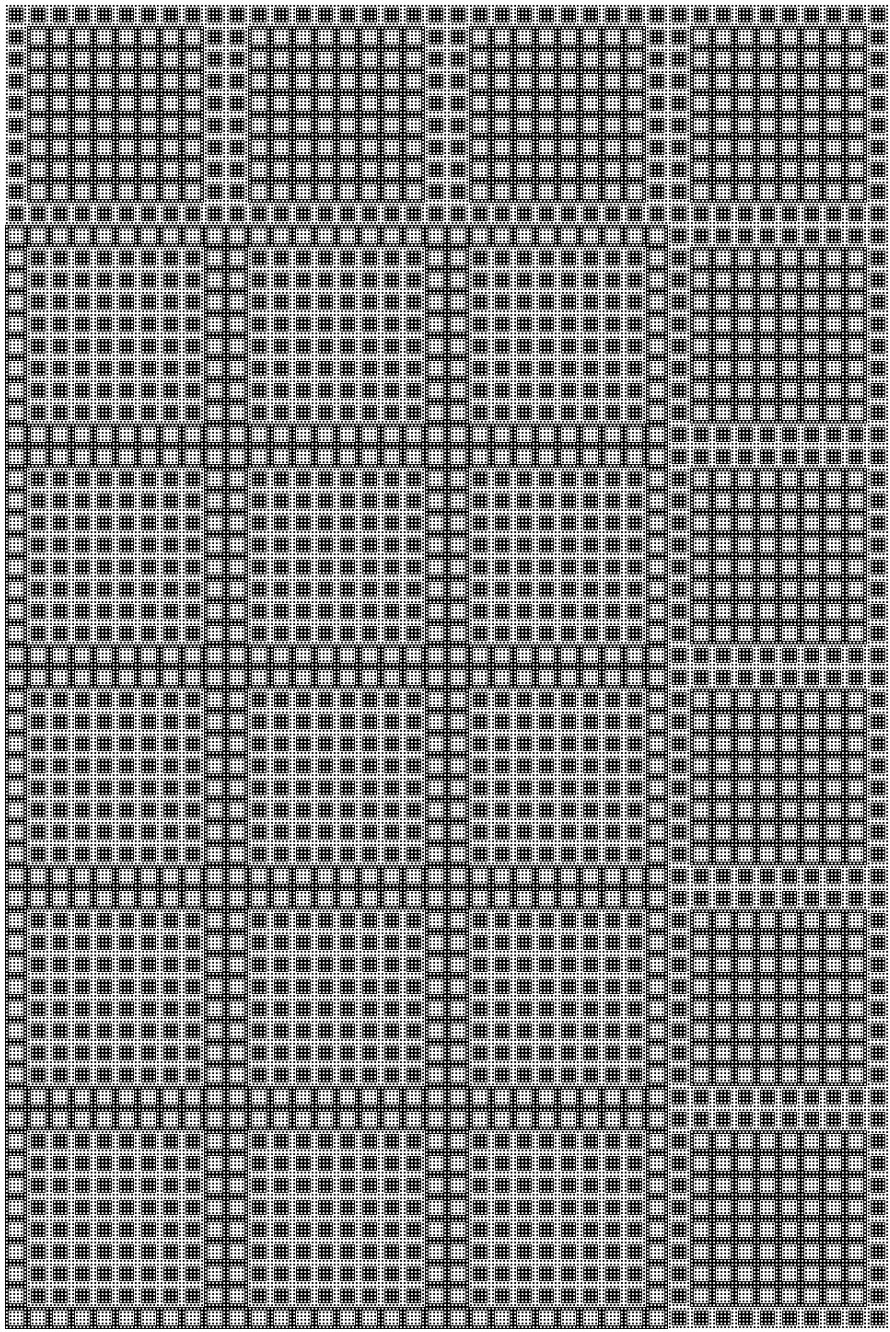


FIGURE 1.13.2. Part of the patch $P_4(1)$ of the fusion rule of Figure 1.13.1.

Several further interesting examples might arise from similar fusion rules. This huge field remains to be explored further.

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CHAPTER 2

Discrete Tomography of Model Sets: Reconstruction and Uniqueness

Uwe Grimm, Peter Gritzmann and Christian Huck

In this chapter, we study the discrete inverse problem of reconstructing finite subsets of $\mathbb{Z}$-modules in Euclidean d-space from their k-dimensional discrete X-rays with respect to finitely many linear subspaces. We are particularly interested in the computational complexities of the related algorithmic problems and in conditions that guarantee uniqueness of the data. These questions have been studied thoroughly for lattices. Here, our focus lies on extensions to Euclidean model sets or quasicrystals.

2.1. Introduction

Discrete tomography (DT) is concerned with the inverse problem of retrieving information about some *finitely* representable object in the Euclidean vector space $\mathbb{R}^d$ from information about its intersections with certain *query sets*. Of particular interest is the problem of *reconstructing* some (or all) finite point sets F from given X-rays $X_{S_1}(F), \ldots, X_{S_m}(F)$ parallel to a small number m of k-dimensional subspaces $S_1, \ldots, S_m$. More precisely, an *X-ray*[1] $X_{S_i}(F)$ of F is the *sum function* parallel to the subspace S_i, which means that it gives the number of points of F on *each* k-dimensional affine space T parallel to S_i. As will become obvious from our explanations below, the special case $k = 1$ of *line X-rays* is of great importance in practical applications; see Figure 2.1.1 for an illustration.

A general problem of great interest is that of *uniqueness*: Does the given X-ray information suffice to determine the set F uniquely? One motivation for studying problems in DT comes from the requirement in materials science for the reconstruction, at the atomic level, of solid state materials from their images under quantitative *high resolution transmission electron microscopy*

[1]The notion of X-rays is meant generically without reference to any imaging technique. In particular, it should not be confused with the same term in Röntgen radiation. The term will be defined more precisely in Definition 2.2.1 below.

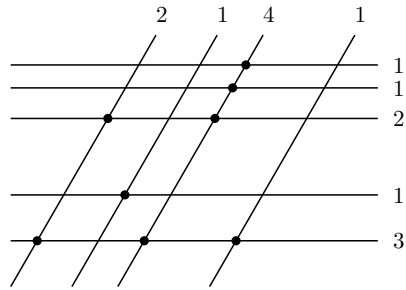

FIGURE 2.1.1. A finite point set (black dots) and its line X-rays in two directions.

(HRTEM). In fact, in [41, 49], a technique is described which can, for certain crystals, effectively measure the number of atoms lying along densely occupied columns. Apparently, for these and many other practical purposes, the basic forms of the DT-problems outlined above have to be adapted to be able to cope with noisy measurements.

While the best-studied case is that of subsets of a lattice L, there is growing interest in the determination of finite subsets of a fixed (and sufficiently nice) Delone set $\varLambda$ that is accessible only through X-rays in a given number m of lines spanned by interpoint (or difference) vectors of $\varLambda$, the so-called *$\varLambda$-lines*. It is motivated by the desire to reconstruct also more general solid state materials such as *quasicrystals* by means of HRTEM measurements.

In this contribution, we will give an account of the computational complexity for various algorithmic tasks in DT, and also address general criteria for uniqueness. We will survey known results in some generality, but usually refer to the original articles for the proofs. Particular emphasis will be placed on the case of (mathematical) quasicrystals.

In the quasicrystallographic setting, the points to be determined belong to a fixed two- or three-dimensional *model set*; compare [9, 42] as well as [AO1, Ch. 7] for a general exposition. Just like lattices, model sets possess a dimensional hierarchy; compare [AO1, Rem. 3.8]. In particular, model sets in 3-space allow a slicing into planar model sets. However, the slices are in general no longer pairwise congruent or equally spaced in 3-space [44]. Still, most of the model sets that describe real quasicrystallographic structures allow a slicing such that each slice is, when seen from a common perpendicular viewpoint, a model set with (statistical) pentagonal, decagonal, octagonal or dodecagonal rotational symmetry; see [31, Sec. 1.2] and [35, Sec. 4.5] as well as [33, 50] for details, and [AO1, Sec. 5.6] for a discussion of the proper notion of symmetry in this context. The latter are examples of *cyclotomic model sets* [AO1, Sec. 7.3], which take over the role played by planar lattices in the crystallographic case.

2.2. Basic notions of discrete tomography

We begin by introducing the basic definitions of discrete tomography in the generality needed subsequently. Let $d \in \mathbb{N}$, $D \subset \mathbb{R}^d$ and $C \subset \mathbb{R}$. For $m \in \mathbb{N}$, we will often use the notation

$$[m] = \{1, \ldots, m\}.$$

Our objects will be functions $\psi\colon D \longrightarrow C$ with domain D and codomain C whose support $\mathrm{supp}(\psi) = \{x \in D \mid \psi(x) \neq 0\}$ is a finite set. In terms of the results available in the literature, the most relevant domain is $D = \mathbb{Z}^d$ for some integer $d \geqslant 2$. Of particular interest in the present context is also the more general situation where D is a finitely generated $\mathbb{Z}$-module of rank d, embedded in Euclidean space. Standard choices for C are $\{0,1\}$, $\mathbb{N}_0$, $\mathbb{Z}$ and the corresponding relaxations $[0,1]$, $[0,1] \cap \mathbb{Q}$, $\mathbb{Q}_{\geqslant 0}$, $\mathbb{R}_{\geqslant 0}$ and $\mathbb{R}$, where $\mathbb{Q}_{\geqslant 0}$ and $\mathbb{R}_{\geqslant 0}$ denote the non-negative rationals and reals, respectively. For any such pair (D, C), let $\mathcal{F}(D, C)$ denote the class of all functions $\psi\colon D \longrightarrow C$ with finite support. Of course, for $C = \{0,1\}$, such a function ψ can be viewed as the indicator function of a finite set F and can be identified with $\mathrm{supp}(\psi)$. Hence, the case $(D, C) = (\mathbb{Z}^d, \{0,1\})$ encodes the classical *finite lattice sets*, and we will write $\mathcal{F}^d$ as an abbreviation for $\mathcal{F}(\mathbb{Z}^d, \{0,1\})$.

For $k \in \mathbb{N}$ with $k \leqslant d-1$, let $\mathcal{S}_{k,d}$ denote the set of all k-dimensional subspaces of $\mathbb{R}^d$, while $\mathcal{S}_{k,d}(D)$ is the subset of $\mathcal{S}_{k,d}$ of those subspaces spanned by vectors of the difference set[2] $D - D$ of D. In particular, $\mathcal{L}_{k,d} = \mathcal{S}_{k,d}(\mathbb{Z}^d)$ is the set of k-dimensional *lattice spaces*. For $S \in \mathcal{S}_{k,d}$, we use the notation $\mathcal{A}(S)$ for the set of all k-dimensional affine subspaces of $\mathbb{R}^d$ that are parallel to S. The situation of $(\mathcal{F}^d, \mathcal{L}_{k,d})$ will be referred to as the *lattice case*.

Definition 2.2.1. Let $\psi \in \mathcal{F}(D, C)$ and $S \in \mathcal{S}_{k,d}$. The *discrete k-dimensional X-ray of ψ parallel to S* is the function $X_S\psi\colon \mathcal{A}(S) \longrightarrow \mathbb{R}$ defined by

$$T \longmapsto \big(X_S\psi\big)(T) = \sum_{x \in T} \psi(x).$$

As above, ψ has finite support, hence all sums are finite.

The mapping $\mathcal{X}_\psi$ on $\mathcal{S}_{k,d}$ defined by $S \mapsto X_S\psi$ is called the *discrete k-dimensional X-ray transform* of ψ. For $k = 1$, it is the standard *discrete X-ray transform* involving *line X-rays*, while for $k = d-1$, it is called the *discrete Radon transform* of ψ whose measurements come from *hyperplane X-rays*.

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[2] If D is an additive group, one certainly has $D - D = D$, but we shall also meet cases where D is just any locally finite point set. In the latter case, $D - D := \{x - y \mid x, y \in D\}$ is known as the *Minkowski difference* of D; compare [AO1, p. 11].

The basic task of DT is to infer information about an unknown function $\psi \in \mathcal{F}(D, C)$ from its X-rays with respect to a finite number m of given spaces $S \in \mathcal{S}_{k,d}$. The affine spaces $T \in \mathcal{A}(S)$ can be parametrised by vectors $t \in S^{\perp}$ such that $T = t + S$. Hence, we may regard $X_S\psi$ as a function on $S^{\perp}$, and accordingly represent measurements by means of *data functions* $f_S \colon S^{\perp} \longrightarrow \mathbb{R}$ with finite support. For algorithmic purposes, we will often use redundant representations $f_S \colon K \longrightarrow \mathbb{R}$ with $K \subset D$ in order to represent the relevant translates of S by translation vectors from D.

2.3. Algorithmic issues in discrete tomography

Here, we will introduce basic algorithmic problems of DT in detail and indicate their structure by formulations that place them into the realm of mathematical optimisation. DT problems have received much attention — with a particular focus on sets contained in $\mathbb{Z}^d$ accessible only through their one-dimensional X-rays in a given finite number m of integer directions; see the survey articles [24, 17, 28] and the monograph [30].

If the subsets are restricted to $\mathbb{Z}^d$ and the subspaces for taking X-rays are generated by integer (or rational) vectors, computational issues can naturally be studied in the well-known *binary Turing machine model*; see [21, 40, 43] for background information. In particular, we assume the reader to be familiar with the basic notions of complexity theory as described in these references. For the binary Turing machine model, an elaborate *non-tractability* theory is available. Particularly, the concepts of $\mathbb{NP}$-*hardness* and $\mathbb{NP}$-*completeness* are powerful tools for showing the *relative* hardness of certain computational problems.[3] Hence, whenever possible (and particularly in Section 2.4), we will adopt the binary Turing machine model.

However, for certain problems involving quasicrystals, we will need the computational power of real number computations. Then, we will use the *real RAM model* to give some tractability results. This will be done in Section 2.5. Unfortunately, this model does not provide a similarly well developed path to intractability results. Section 2.5 will, however, indicate the computational difficulties of discrete tomography over $\mathbb{Z}$-modules. This is the situation for all quasicrystals of practical relevance.

2.3.1. Basic algorithmic tasks

Let $d, k, m \in \mathbb{N}$ with $2 \leqslant d, m$ and $k \leqslant d - 1$. Also, let $S_1, \ldots, S_m$ be m distinct elements of $\mathcal{S}_{k,d}$. One of the basic problems is the *consistency* of the setting, which can be formulated as follows.

[3] Recall that the open *millennium problem* '$\mathbb{P} = \mathbb{NP}$?' asks whether the relative notion of $\mathbb{NP}$-hardness indeed constitutes an absolute classification.

CONSISTENCY$_{\mathcal{F}(D,C)}(S_1, \dots, S_m)$.
Instance: *Data functions* $f_{S_1}, \dots, f_{S_m}$.
Question: *Does there exist a function* $\psi \in \mathcal{F}(D, C)$ *such that* $X_{S_i}\psi = f_{S_i}$ *for all* $i \in [m]$*?*

In the following, when $S_1, \dots, S_m$ are given, we will often write f_i for f_{S_i} to simplify the notation. Note that, for any given instance $\mathcal{I} = (f_1, \dots, f_m)$ of CONSISTENCY$_{\mathcal{F}(D,C)}(S_1, \dots, S_m)$, the support of any solution is contained in the *grid*

$$G = G(\mathcal{I}) = \bigcap_{i=1}^{m} \big(\operatorname{supp}(f_i) + S_i\big)$$

associated with $\mathcal{I}$. The grid $G(\mathcal{I})$ can be computed from the sets $\operatorname{supp}(f_i)$ with $i \in [m]$ by solving polynomially many systems of linear equations.

Of course, any solution of CONSISTENCY$_{\mathcal{F}(D,C)}(S_1, \dots, S_m)$ is not just contained in G but, by definition, also in D. There are, however, situations where the position of D relative to the measurements is not precisely known. For quasicrystals, for instance, it is not clear where such a solution may exist in the underlying structure. Hence, the *anchored* problem CONSISTENCY$_{\mathcal{F}(D,C)}(S_1, \dots, S_m)$ is a special case of a more general problem which is defined relative to a set Φ of transformations of $\mathbb{R}^d$.

CONSISTENCY$_{\mathcal{F}(D,C)}(\Phi, S_1, \dots, S_m)$.
Instance: *Data functions* $f_1, \dots, f_m$.
Question: *Do there exist functions* $\psi \in \mathcal{F}(D, C)$ *and* $\varphi \in \Phi$ *such that* $X_{S_i}(\varphi \circ \psi) = f_i$ *for all* $i \in [m]$*?*

Most important and best studied is the anchored case where Φ just consists of the identity. Due to its relevance for quasicrystals, the second most important choice for Φ is the set Γ of translations of $\mathbb{R}^d$; see [7], where the problem was first introduced, and [25]. Note that, since the X-rays are parallel to the given subspaces, the potential restriction $S_1, \dots, S_m \in \mathcal{S}_{k,d}(D)$ is not affected when D is only fixed up to translations.

There are, however, other reasonable choices like, for instance, the set of rigid motions in $\mathbb{R}^d$. In colloquial terms, rigid motions reflect the fact that looking at a photograph or slide (visible from both sides) anywhere in space does not change the shown image. In such cases, the restriction of X-ray images to lines spanned by vectors in D leads to the additional restrictions on Φ that the preimages of $S_1, \dots, S_m$ are spanned by vectors in D.

Below, we will mostly concentrate on the anchored case. In Section 2.5, we will discuss additional problems that originate for $\Phi = \Gamma$ in the context of quasicrystals. In particular, we will identify tasks that reflect the fact that only certain subsets of a given $\mathbb{Z}$-module are allowed. For simplicity,

we refrain from introducing our task in full generality. It is, however, always straightforward to add the set Φ when required.

From a practical point of view, it is more relevant to actually *reconstruct* a solution rather than to just ask for its existence.

$\textsc{Reconstruction}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$.
Instance: *Data functions* $f_1, \ldots, f_m$.
Task: *Determine a function* $\psi \in \mathcal{F}(D,C)$ *such that* $X_{S_i}\psi = f_i$ *for all* $i \in [m]$*, or decide that no such function exists.*

Clearly, $\textsc{Reconstruction}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$ cannot be easier than deciding feasibility, i.e., $\textsc{Consistency}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$.

Another important algorithmic task involves verifying the *uniqueness* of a solution.

$\textsc{Uniqueness}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$.
Instance: *A function* $\psi \in \mathcal{F}(D,C)$.
Question: *Does there exist* $\psi' \in \mathcal{F}(D,C) \setminus \{\psi\}$ *such that* $X_{S_i}\psi = X_{S_i}\psi'$ *for all* $i \in [m]$*?*

Apparently, the two problems of $\textsc{Consistency}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$ and of $\textsc{Uniqueness}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$ are special cases of (and hence no harder than) the corresponding *counting problem*.

$\#\textsc{Consistency}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$.
Instance: *Data functions* $f_1, \ldots, f_m$.
Task: *Determine the cardinality of the set of functions* $\psi \in \mathcal{F}(D,C)$ *such that* $X_{S_i}\psi = f_i$ *for all* $i \in [m]$.

Note that, for $S \in \mathcal{S}_{1,d} \setminus \mathcal{S}_{1,d}(D)$, the problems are not particularly interesting. In fact, for each $t \in D$, the line $T = t + S$ then intersects $D \cap G(\mathcal{I})$ in at most one point. Hence, each $\psi \in \mathcal{F}(D,C)$ is determined uniquely by just one line X-ray parallel to $S \in \mathcal{S}_{1,d} \setminus \mathcal{S}_{1,d}(D)$. The same is true for each $S \in \mathcal{S}_{k,d}$ with the property that

$$\operatorname{card}\bigl(T \cap D \cap G(\mathcal{I})\bigr) \leqslant 1 \quad \text{for each } T \in \mathcal{A}(S).$$

If all $S_1, \ldots, S_m \in \mathcal{S}_{k,d} \setminus \mathcal{S}_{k,d}(D)$ contain non-trivial subspaces spanned by vectors from $D - D$, the situation changes. As we shall see in Section 2.5.1, this is the case for quasicrystals. We will usually, and in particular in all of Section 2.4, assume that all spaces are spanned by vectors from $D - D$, so that $S_1, \ldots, S_m \in \mathcal{S}_{k,d}(D)$.

Clearly, if the set ψ of functions is a solution for a given instance $\mathcal{I}$ of $\textsc{Consistency}_{\mathcal{F}^d(D,C)}(S_1,\dots,S_m)$, its *total weight*

$$\|\psi\|_{(1)} = \sum_{x\in D} |\psi(x)|$$

equals $\|f_i\|_{(1)}$ for all $i \in [m]$. Consequently,

$$\|f_1\|_{(1)} = \dots = \|f_m\|_{(1)}$$

is a necessary condition for consistency. Since this condition can be checked efficiently (if, as we always assume, the functions can be computed efficiently), we will generally *assume* that it is satisfied, and set $n = n(\mathcal{I}) = \|f_1\|_{(1)}$.

In order to derive results on the algorithmic properties of these (and other) problems, we have to specify the models of computation we want to employ. This means that we need to define which computational power is presupposed and how the algorithmic effort is measured. As mentioned above, we shall use the two most standard frameworks, the binary Turing machine model and the real RAM model.

2.3.2. Optimisation models

It is quite natural to try to model the two related (anchored) problems, $\textsc{Reconstruction}_{\mathcal{F}(D,C)}(S_1,\dots,S_m)$ and $\textsc{Consistency}_{\mathcal{F}(D,C)}(S_1,\dots,S_m)$, as finite-dimensional feasibility problems (asking for a solution or just the existence of a solution). Using variables $\xi_x \in C$ associated with the grid points $x \in G \cap D$ of a given instance $\mathcal{I}$, one may write

$$\sum_{x\in T\cap G} \xi_x = f_i(T) \quad \text{for } i \in [m] \text{ and } T \in \mathcal{A}(S_i).$$

Note, however, that $G \cap D$ need not always be finite. This may seem a mere technical problem, but it is not.

To illustrate this point, let us consider the reconstruction problem, restricted to a simple one-parameter family of instances $\mathcal{I}_n$ for $n \in \mathbb{N}$ of the lattice case for $k = 2$ and $d = 3$, where S_1 and S_2 denote the two coordinate planes of $\mathbb{R}^3$ parallel to the third axis. To define $\mathcal{I}_n$, set

$$f_i(T) = \begin{cases} n, & \text{for } T = S_i, \\ 0, & \text{for } T \in \mathcal{A}(S_i) \setminus \{S_i\}, \end{cases} \qquad \text{for } i \in \{1,2\}.$$

These instances of $\textsc{Reconstruction}_{\mathcal{F}^3(S_1,S_2)}$ are utterly trivial: Simply place n points on the third coordinate axis. In the binary Turing machine model, the *size* of a given instance $\mathcal{I}$, denoted by $\operatorname{size}(\mathcal{I})$, is the total number of bits needed to encode the data. The bit length of the data functions f_1 and f_2 is therefore based on the *logarithm* of the values, not on the values themselves. Hence, each instance $\mathcal{I}_n$ can be encoded by a constant number

of bits for the set-up and $O(\log(n))$ bits[4] for the single non-zero value of each function f_i. Consequently, in the binary Turing machine model, the trivial algorithm has an exponential running time. Even worse, each solution consists of n points and is hence exponential in size($\mathcal{I}$), which means that the problem itself, albeit trivial, does not even admit polynomial-space solutions.

The situation changes, however, if we restrict the admissible instances $\mathcal{I}$ to those whose cardinality $n(\mathcal{I})$ is bounded by a polynomial in size($\mathcal{I}$). This is certainly guaranteed if we assume that the grids $G(\mathcal{I})$ are finite. Then, the coefficient matrix of the above system of linear equations is a 0-1-matrix of size bounded by a polynomial in the input. Note that G is indeed always finite for line X-rays. Unless stated otherwise, we assume G to be *finite* from now on.

Given a function $\psi \in \mathcal{F}(D, C)$ that specifies an instance of UNIQUENESS$_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$, one can decide whether there exists another solution ψ' by solving another optimisation problem. In fact, with $\|\psi\|_{(2)}^2 = \sum_{x\in D} \psi(x)^2$, we have

$$\|\psi - \psi'\|_{(2)}^2 \;=\; \|\psi\|_{(2)}^2 + \|\psi'\|_{(2)}^2 - 2\sum_{x\in G} \psi(x)\psi'(x).$$

Hence, maximising the distance of a solution to the given one can be expressed as the following optimisation problem in the variables $\xi_x \in C$ with $x \in G$,

$$\min \sum_{x\in G} \psi(x)\,\xi_x \quad \text{subject to} \quad \sum_{x\in T\cap G} \xi_x \;=\; f_i(T) \quad \text{for } i \in [m],\, T \in \mathcal{A}(S_i).$$

Note that, for $C \in \{[0,1], [0,1]\cap\mathbb{Q}, \mathbb{Q}_{\geqslant 0}, \mathbb{R}_{\geqslant 0}, \mathbb{R}\}$, the optimisation problems boil down to linear programming, while $C \in \big\{\{0,1\}, \mathbb{N}_0\big\}$ confronts us with *integer* linear programming. For $C = \mathbb{Z}$, the tasks involve the solution of a system of linear Diophantine equations.

2.4. Computational complexity of discrete tomography

In the binary Turing machine model, all explicitly encoded data must have finite bit length. For the purposes of this section, we will therefore restrict the data to be rational, so $D \subset \mathbb{Q}^d$, $C \subset \mathbb{Q}$ and $S \in \mathcal{L}_{k,d}$.

The spaces $S \in \mathcal{L}_{k,d}$ can be parametrised by specifying k vectors $v_j \in \mathbb{Z}^d$ with $j \in [k]$ that span S or, alternatively, by means of selecting $n-k$ vectors $a_i \in \mathbb{Z}^d$ with $i \in [n-k]$ such that S is the solution space of the linear system $a_i^T x = 0$ with $i \in [n-k]$. Naturally, the former is generally more adequate for line X-rays, while the latter is preferred for hyperplane X-rays. Each relevant space $T \in \mathcal{A}(S)$ can then be represented by a vector $t \in G$

[4]Note that $O(f(n))$ refers to the standard order notation due to Landau, which specifies an asymptotic upper bound as $n \to \infty$.

such that $T = t + S$. Of course, this encoding is generally not unique, but has the advantage that the representation of the data functions can be linked to the grid G associated with the input. For more information on adequate data structures, see [19] where details are given for one-dimensional X-rays of lattice sets, which readily extend to full generality.

Under the general assumption that the grid $G(\mathcal{I})$ is finite, both problems, $\textsc{Consistency}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$ and $\textsc{Uniqueness}_{\mathcal{F}(D,C)}(S_1, \ldots, S_m)$, belong to the class $\mathbb{NP}$. (Note that the latter checks, in effect, non-uniqueness to put this problem into $\mathbb{NP}$ rather than into co$\mathbb{NP}$.)

Recall from Section 2.3.2 that, for the codomains $[0, 1]$, $[0, 1] \cap \mathbb{Q}$ and $\mathbb{Q}_{\geqslant 0}$, our problems $\textsc{Consistency}_{\mathcal{F}^d(\mathbb{Z}^d,C)}(S_1, S_2)$, $\textsc{Uniqueness}_{\mathcal{F}^d(\mathbb{Z}^d,C)}(S_1, S_2)$ and $\textsc{Reconstruction}_{\mathcal{F}^d(\mathbb{Z}^d,C)}(S_1, S_2)$ can be solved by linear programming and hence efficiently; compare [48]. Let us note in passing that the counting problem $\#\textsc{Consistency}_{\mathcal{F}^d(D,C)}(S_1, \ldots, S_m)$ is essentially meaningless for these codomains since a given instance permits either no, one, or infinitely many solutions, as the set of all solutions in $\mathcal{F}(D, \mathrm{cl}(C))$ (i.e., with values in the closure of C) is convex.

For $C = \mathbb{Z}$, we need to solve a system of linear Diophantine equations which can also be done in polynomial time with the aid of the *Hermite normal form*; see [48]. Hence, we will focus on the codomains $\{0, 1\}$ and $\mathbb{N}_0$.

In the remainder of this section, we will state the results for $D = \mathbb{Z}^d$. Note that this situation comprises both the problem of reconstructing lattice subsets from their line X-rays ($D = \mathbb{Z}^d, C = \{0, 1\}$) and the problem from statistics of reconstructing non-negative integer contingency tables from certain marginal sums ($D = \mathbb{Z}^d, C = \mathbb{N}_0$); see [38] for details.

2.4.1. Line X-rays

Let us continue with an overview of the results about the computational complexity of the above tasks for one-dimensional X-rays. The first result concerns the case $m = 2$.

Theorem 2.4.1 ([46]). *If $S_1, S_2 \in \mathcal{L}_{1,d}$ are different sets, all three problems, $\textsc{Consistency}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, S_2)$, $\textsc{Uniqueness}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, S_2)$ as well as $\textsc{Reconstruction}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, S_2)$, can be solved in polynomial time, both for $C = \{0, 1\}$ and for $C = \mathbb{N}_0$.* □

Note that the question for the computational complexity of $\#\textsc{Consistency}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, S_2)$ remains open. For $C = \{0, 1\}$, Theorem 2.4.1 was proved combinatorially in [46] (see also [47]), while [23] evokes network optimisation. The theorem follows easily from the fact that, when formulated as integer linear programs, the tasks involve a *totally unimodular* coefficient

matrix and can therefore be solved as linear programs; see for instance [48] for more information about total unimodularity and its consequences.

The next results for $m \geqslant 3$ are due to [19, Thms. 3.7 and 4.3, Cor. 3.8]; see also [27, Thm. 2.1] for a slight extension.

Theorem 2.4.2 ([19]). *Let $m \geqslant 3$, and let $S_1, \ldots, S_m \in \mathcal{L}_{1,d}$ be m distinct lattice lines. Then, the two problems* $\textsc{Consistency}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, \ldots, S_m)$ *and* $\textsc{Uniqueness}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, \ldots, S_m)$ *are $\mathbb{NP}$-complete, while* $\textsc{Reconstruction}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, \ldots, S_m)$ *is $\mathbb{NP}$-hard in the strong sense for $C = \{0, 1\}$ and $C = \mathbb{N}_0$. Further,* $\#\textsc{Consistency}_{\mathcal{F}^d(\mathbb{Z}^d,C)}(S_1, \ldots, S_m)$ *is $\#\mathbb{P}$-complete.* □

In fact, it was actually shown in [19] that the statements for $C = \{0, 1\}$ remain true even when restricted to instances where two of the data functions f_i take values in $\{0, 1\}$ only. This observation then immediately implies the intractability results for $C = \mathbb{N}_0$ because such instances permit only solutions ψ with values in $\{0, 1\}$.

In [12], Theorem 2.4.2 was refined to even more restrictive classes of instances, allowing also hardness results for the reconstruction of binary and permutation matrices. In view of Theorem 2.4.2, one may wonder whether the problems become easier if the requirement on fitting the data is relaxed. More specifically, let us consider the following problems.

X-ray-$\textsc{Correction}_{\mathcal{F}^d}(S_1, \ldots, S_m)$.
Instance: *Data functions $f_1, \ldots, f_m$.*
Question: *Does there exist $F \in \mathcal{F}^d$ such that $\sum_{i=1}^m \|X_{S_i} F - f_i\|_{(1)} \leqslant m - 1$?*

$\textsc{Similar-Solution}_{\mathcal{F}^d}(S_1, \ldots, S_m)$.
Instance: *A set $F_1 \in \mathcal{F}^d$.*
Question: *Does there exist $F_2 \in \mathcal{F}^d$ with $|F_1| = |F_2|$ and $F_1 \neq F_2$ such that $\sum_{i=1}^m \|X_{S_i} F_1 - X_{S_i} F_2\|_{(1)} \leqslant 2m - 3$?*

Let us point out that these two problems are specialisations of problems for which an additional error term is part of the input. They are presented with the specific bounds $m - 1$ and $2m - 3$ to formulate the next theorem as sharply as possible. In fact, while $\textsc{Consistency}_{\mathcal{F}^d}(S_1, \ldots, S_m)$ is highly ill-posed in general [4], it does nevertheless feature some limited stability [1, Thm. 2.1]. This can be used to derive the following complexity results.

Theorem 2.4.3 ([1]). *Let $S_1, \ldots, S_m \in \mathcal{L}_{1,d}$ be distinct. Then, the problems* X-ray-$\textsc{Correction}_{\mathcal{F}^d}(S_1, \ldots, S_m)$ *and* $\textsc{Similar-Solution}_{\mathcal{F}^d}(S_1, \ldots, S_m)$ *are in $\mathbb{P}$ for $m \leqslant 2$, but are $\mathbb{NP}$-complete for $m \geqslant 3$.* □

For some tractability results for weaker forms of approximation, see [29]. Theorem 2.4.3 says that lifting the condition of perfect fit only by the constants $m-1$ or $2m-3$, respectively, is simply not enough to render the problems easy. Actually, in some sense, the situation is much worse. As shown in [26], DT for $m \geqslant 3$ is somehow trapped by the impossibility of combining reasonable approximation with high computational speed. This shows the particular limitations of large classes of obvious approaches that utilise the fact that the underlying problems can be solved efficiently when only information in two directions is given.

Let us give an example of one such procedure for $m = 3$ and distinct lines $S_1, S_2, S_3 \in \mathcal{L}_{1,d}$. We begin by reconstructing a solution $F_{1,2}$ for the corresponding instance of $\textsc{Reconstruction}_{\mathcal{F}^d}(S_1, S_2)$. Then, we solve the instance of $\textsc{Reconstruction}_{\mathcal{F}^d}(S_1, S_3)$ with the additional requirement that, among all solutions, the obtained one must be closest to $F_{1,2}$. Using the framework of Section 2.3.2, this can be done in polynomial time.

The process can now be iterated by replacing the current 2-element subset of $\{S_1, S_2, S_3\}$ by any other until some stopping rule applies. Note that, if the given instance is consistent, the resulting set F satisfies at least the conditions for the two directions employed in the final step. Hence, this algorithm solves the following problem.

2-Exact-Maximum-Constraint-Fit$_{\mathcal{F}^d}(S_1, S_2, S_3)$.

Instance: *Data functions* f_1, f_2, f_3.

Task: *Find a set* $F \subset G$ *with* $X_{S_i} F(T) = f_i(T)$ *for all* $T \in \mathcal{A}(S_i)$ *and* $i \in \{1, 2\}$ *such that* F *maximises* $\operatorname{card}\big(\{T \in \mathcal{A}(S_3) \mid X_{S_3} F(T) = f_3(T)\}\big)$.

The next result highlights the inherent difficulties of this problem.

Theorem 2.4.4 ([26])**.** *Let* $S_1, S_2, S_3 \in \mathcal{L}_{1,d}$ *be distinct. Then, there exists a constant* ρ *with* $\rho < 1$ *such that, unless* $\mathbb{P} = \mathbb{NP}$*, no polynomial time algorithm can approximate* 2-Exact-Maximum-Constraint-Fit$_{\mathcal{F}^d}(S_1, S_2, S_3)$ *with performance guarantee* ρ*, that is, with an output not below* ρ *times the optimum.* □

As it turns out, not even the knowledge of a large part of a solution is of much help. The following result is based on a modification of a construction given in [19].

Theorem 2.4.5 ([26])**.** *Let* $m \geqslant 3$ *and let* $S_1, \ldots, S_m \in \mathcal{L}_{1,d}$ *be distinct. Further, let* $0 < \varepsilon \leqslant 1$*. Unless* $\mathbb{P} = \mathbb{NP}$*, there is no polynomial time algorithm to solve the reconstruction problem even if all but* n^{ε} *out of* n *points are known beforehand.* □

There are various applications of DT in physics and materials science. A particularly interesting problem is that of tracking particles over time; see [3, 52]. As it turns out, in contrast to the results of Theorem 2.4.1, some such problems are $\mathbb{NP}$-hard even in the case $m = 2$; see [2] and the papers quoted there.

Let us close this section by mentioning a tractability result from [10] for the reconstruction of *convex* lattice sets, which are sets $F \subset \mathbb{Z}^d$ such that

$$F \;=\; \mathrm{conv}(F) \cap \mathbb{Z}^d.$$

This class is particularly relevant in view of the uniqueness theorem of [16] whose generalisation to convex subsets of algebraic Delone sets is at the heart of Section 2.6.2. Reference [10] shows that, for sets of four lattice directions that satisfy the criterion of [16], convex lattice sets can actually be reconstructed in polynomial time.

2.4.2. Higher-dimensional X-rays

The case of higher-dimensional X-rays has not been studied as comprehensively as that of one-dimensional X-rays. In fact, some additional features occur that make the problems more difficult to handle. For instance, it has been shown in [27] that, even though there is an obvious geometric duality between lines and hyperplanes, the case of Radon transforms is much more involved than that of the standard X-ray problems: Various phenomena occur for $k = d - 1$ that are absent for $k = 1$. In particular, it is generally not only the parameters d and m that determine the computational complexity, but also the intersection pattern of the hyperplanes. The following result contains some tractable cases.

Theorem 2.4.6 ([18])**.** *Let $S_1, S_2 \in \mathcal{L}_{k,d}$. Then, under the restriction that, for any instance $\mathcal{I}$, the cardinality $n(\mathcal{I})$ is bounded by a polynomial in the bit length of the data functions, the problems* $\textsc{Consistency}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, S_2)$, $\textsc{Uniqueness}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, S_2)$ *as well as* $\textsc{Reconstruction}_{\mathcal{F}(\mathbb{Z}^d,C)}(S_1, S_2)$ *can be solved in polynomial time for $C = \{0, 1\}$ and for $C = \mathbb{N}_0$.* □

Unsurprisingly, the hardness results of Theorem 2.4.2 can be utilised to obtain some hardness results for larger k; compare [17, Thm. 4.5.2]. The first intrinsically 2-dimensional transformation in $\mathbb{R}^3$ is due to [11]. Let $S_1^d, \ldots, S_d^d$ denote the coordinate hyperplanes in $\mathbb{R}^d$. Then, [11, Thm. 3.3] determines the computational complexity of $\textsc{Consistency}_{\mathcal{F}^3}(S_1^3, S_2^3, S_3^3)$. The other results of the following theorem are taken from [27, Thm. 2.7].

Theorem 2.4.7. *For any fixed $d = m \geqslant 3$,* $\textsc{Consistency}_{\mathcal{F}^d}(S_1^d, \ldots, S_d^d)$ *and* $\textsc{Uniqueness}_{\mathcal{F}^d}(S_1^d, \ldots, S_d^d)$ *are $\mathbb{NP}$-complete in the strong sense, while* $\#\textsc{Consistency}_{\mathcal{F}^d}(S_1^d, \ldots, S_d^d)$ *is $\#\mathbb{P}$-complete.*

For the codomains $[0,1] \cap \mathbb{Q}$ *and* $\mathbb{Q}_{\geqslant 0}$*, the two problems* Consistency$_{\mathcal{F}^d}(S_1^d, \ldots, S_d^d)$ *and* Uniqueness$_{\mathcal{F}^d}(S_1^d, \ldots, S_d^d)$ *can be solved in strongly polynomial time.* □

Using techniques from [12], one can readily extend Theorem 2.4.7 to larger generality. Let us further point out that Theorem 2.4.7 shows that, unless $\mathbb{P} = \mathbb{NP}$, there is no theoretical consistency or uniqueness condition for $d = m \geqslant 3$ and $C = \{0,1\}$ that can be checked efficiently.

As Theorems 2.4.1 and 2.4.2 show, the computational complexity for $k = 1$ does not change if we move from $C = \{0,1\}$ to $C = \mathbb{N}_0$. It may therefore come as a surprise that the $\mathbb{NP}$-hardness results of Theorem 2.4.7 do *not* extend to $C = \mathbb{N}_0$. In fact, using algebraic methods, [51, Sec. 4.2.2] gave the following tractability result; the subsequent characterisation of feasibility (which yields an elementary algorithm) can be found in [27, Sec. 4].

Theorem 2.4.8. *The two problems* Consistency$_{\mathcal{F}(\mathbb{Z}^d,\mathbb{N}_0)}(S_1^d, \ldots, S_d^d)$ *and* Uniqueness$_{\mathcal{F}(\mathbb{Z}^d,\mathbb{N}_0)}(S_1^d, \ldots, S_d^d)$ *can be solved in polynomial time.*

Furthermore, a given instance $\mathcal{I} = (f_{S_1^d}, \ldots, f_{S_d^d})$ *of the problem* Consistency$_{\mathcal{F}(\mathbb{Z}^d,\mathbb{N}_0)}(S_1^d, \ldots, S_d^d)$ *is feasible if and only if* $\|f_{S_1^d}\|_{(1)} = \ldots = \|f_{S_m^d}\|_{(1)}$ *is satisfied.* □

2.5. Discrete tomography of model sets

From now on, we will leave the results that are tailor-made for the lattice case, and allow D to be any *finitely generated* $\mathbb{Z}$*-module* of rank d. Since our main focus will be on the case of *quasicrystals*, we will concentrate on the codomain $C = \{0,1\}$. As will be made precise below, s-dimensional X-rays of model sets in $\mathbb{R}^r$ correspond naturally to $s + (d-r)$-dimensional X-rays of lattice sets in $\mathbb{R}^d$. The X-ray spaces occurring are, however, not generated by lattice vectors.

2.5.1. Mathematical quasicrystals

Even though model sets have already been introduced in great detail in the first volume of this series [AO1], we will, in the course of the exposition, give a short customised elementary account of those aspects of Euclidean *cut and project schemes* (CPS) that are most relevant in our context. We refer to [AO1, Ch. 7] for a treatment in greater generality. Note that some of the standard notation has been changed to match the existing literature on quasicrystal DT.

Let L be a fixed d-dimensional lattice in $\mathbb{R}^d$, $r \in \mathbb{N}$, $r \leqslant d-1$, and let X be an r-dimensional subspace of $\mathbb{R}^d$ such that $X^\perp \cap L = \{0\}$. Here, X will be regarded as the *physical space* which hosts the quasicrystal, while $Y = X^\perp$

is the *internal space*. Let

$$\varPi_X \colon \mathbb{R}^d \longrightarrow Y, \quad \varPi_Y \colon \mathbb{R}^d \longrightarrow X,$$

denote the projection parallel to X or Y, respectively. Note that the condition $Y \cap L = \{0\}$ implies that the restriction $\varPi_Y|_L$ of $\varPi_Y$ to L is injective. We set

$$D_X \,=\, \varPi_Y(L), \quad D_Y \,=\, \varPi_X(L).$$

Of course, D_X and D_Y are finitely generated $\mathbb{Z}$-modules, and D_X is not discrete in this situation.

Now suppose that m different s-dimensional subspaces $R_1, \ldots, R_m$ of X are given, spanned by vectors of the $\mathbb{Z}$-module D_X, so that $R_i \in \mathcal{S}_{s,r}(D_X)$ for each $i \in [m]$. For these, X-ray images are taken and encoded again by means of data functions $f_{R_i}(z)$. Then, the question of consistency is whether there exists a set $F_X \subset D_X$ whose X-rays with respect to $R_1, \ldots, R_m$ coincide with the given data functions.

We can transform the underlying consistency and reconstruction problem so as to exhibit its relation to the lattice case as follows. Let

$$k \,=\, s + (d - r) \quad \text{and} \quad S_i \,=\, R_i + Y \text{ for } i \in [m].$$

Then, $S_1, \ldots, S_m \in \mathcal{S}_{k,d}$. Since $\varPi_Y|_L$ is injective, the solutions $F_X \subset D_X$ of the original problem are in one-to-one correspondence with the solutions $F \subset L$ of $\textsc{Consistency}_{\mathcal{F}(L,\{0,1\})}(S_1, \ldots, S_m)$. Now, observe that each S_i contains an s-dimensional subspace L_i spanned by vectors of L. Since, for any $g \in L$, one has

$$\operatorname{card}\bigl(F \cap (g + L_i)\bigr) \,=\, \operatorname{card}\bigl(F \cap (g + S_i)\bigr) \,=\, \operatorname{card}\bigl(F_X \cap (\varPi_Y(g) + R_i)\bigr),$$

we can in principle evoke results for the lattice case. Note, however, that neither the instances of the problem in D_X nor the solutions F_X can be finitely encoded in the binary Turing machine model. In general, the sets F and the subspaces $S_1, \ldots, S_m$ are not rational either.

There is, however, an indirect way to encode the data and the solutions appropriately since the lattice L is fixed, and hence not part of the input. In fact, let $a_1, \ldots, a_d$ be a fixed lattice basis for L. With the basis matrix $A = (a_1, \ldots, a_d)$, one then has

$$L \,=\, A\,\mathbb{Z}^d.$$

Then, we can (indirectly) encode each point g of L by the unique integer vector $z \in \mathbb{Z}^d$ such that $g = Az$. Further, suppose that, for each $i \in [m]$, vectors $z_{i,1}, \ldots, z_{i,s} \in \mathbb{Z}^d$ are given explicitly such that

$$g_{i,j} \,=\, Az_{i,j} \quad \text{with } j \in [s]$$

span L_i, and set

$$Z_i \;=\; \mathrm{lin}\big(\{z_{i,1},\dots,z_{i,s}\}\big) \quad \text{for } i\in[m].$$

Then, the instance can be encoded by finite subsets of $\big\{(z,f_{Z_i}(z)) \mid z\in\mathbb{Z}^d\big\}$ where $f_{Z_i}(z)$ is the corresponding measurement for $Az+L_i$.

Note, however, that such an encoding transfers part of the problem into the input. In fact, while the corresponding grid in X may have small diameter, the points z needed for the rational encoding may have large coordinates. Also, as physical measurements take place in X, it is not clear how to actually produce the information in this form.

So far, we have not left the anchored case. This will change now with the final part of the introduction of model sets. Mathematical quasicrystals come with an additional constraint in form of a *window* $W\subset Y$. Let

$$(.)^\star \;=\; \varPi_X\circ {\varPi_Y|_L}^{-1}\colon D_X \longrightarrow D_Y$$

denote the *star map* of the CPS and set

$$\curlywedge(W) \;=\; \{x\in X \mid x^\star\in W\}, \quad \mathcal{M}(W) \;=\; \{t+\curlywedge(W+y) \mid t\in X, y\in Y\}.$$

Then, each element of $\mathcal{M}(W)$ is a *model set* for the CPS $(X,Y;W)$. Note that translations are allowed within X and Y. Hence, we are in the non-anchored case of Section 2.2 involving translations. These translations reflect the situation that, in physical applications, a natural choice of the origin is often impossible (although the rotational orientation of a probe in an electron microscope can, in principle, be determined through diffraction). In colloquial terms, translations in X occur because it might not be clear where in a non-periodic structure a given set might be located, while the translation $y\in Y$ is due to the fact that corresponding structures may only be determined in the limit that the system becomes infinitely large. This problem corresponds to the fact that there may be many different patterns that are *locally indistinguishable* (LI); see [AO1, Ch. 7] for a general discussion of this phenomenon, and see [7] for its relevance to DT.

Even if an accessible encoding of the input is given, it is not clear how to compute a solution. In view of the results of the previous sections, this is not surprising for $m\geqslant 3$. Here, of course, we encounter additional difficulties that already affect the case $m=2$. Even checking the feasibility of a given candidate F_X for a solution for the given instance requires the approximation to finite precision. A thorough study of approximate X-ray problems has not yet been pursued, and would, in any case, be limited by the inherent ill-posedness of DT [4].

Further, the power of an extension to algebraic computations is unclear. Hence, the existing accounts of DT presuppose the power of the real RAM model which allows computations over $\mathbb{R}$. The main focus has been on the

case $m = 2$ and, here, in trying to use real arithmetic in order to preprocess the problem so that standard techniques from the (anchored) lattice case can be applied. To this end, [6, 7] introduced two additional problems, the *decomposition problem* and the *separation problem* that reflect the possible translations, the former in X and the latter in Y, which we now discuss in some detail.

2.5.2. The decomposition problem

As before, let $R_1, \ldots, R_m$ denote m different s-dimensional subspaces of X spanned by vectors from D_X, and let G be the grid associated with a given tomographic instance. For simplicity, suppose that $R_1 \cap \cdots \cap R_m = \{0\}$. This implies that G is finite. In the anchored lattice case with a fixed origin, the computation of solutions can be restricted to $G \cap \mathbb{Z}^d$. In the non-anchored case of model sets, the grid G will generally not be contained in a single translate of D_X, but in a union of several such translates. However, any feasible solution of the underlying reconstruction problem must belong entirely to just one such class. This is, of course, an additional constraint.

Let us mention in passing that this constraint is already relevant in the non-anchored lattice case: There may exist 'solutions' that are not supported by a single translate of the lattice; Figure 2.5.1, taken from [25], illustrates this point in an example.

The *decomposition problem of discrete tomography* now asks whether there is a uniform bound, independent of the solutions F_X, on the number of elements of a partition of the tomographic grid into subsets that are contained in a single translate of the underlying module. Equivalently, this is the question whether the *complete tomographic grid* or *Siegel grid*

$$H = \bigcap_{i=1}^{m} \bigcup_{x \in D_X} (x + R_i)$$

decomposes into finitely many equivalence classes $t + D_X$. This problem has been introduced in [7] and answered in the affirmative for cyclotomic model sets; see [AO1, Sec. 7.3] for background on cyclotomic model sets. More precisely, an n-cyclotomic model set $\varLambda$ lives in the ring of cyclotomic integers $\mathcal{O}_n = \mathbb{Z}[\zeta_n]$, where $n \geqslant 3$ and $\zeta_n = \mathrm{e}^{\frac{2\pi \mathrm{i}}{n}}$; see Section 2.6.2 for some additional algebraic background information. Of course, we need to identify $\mathbb{C}$ with $\mathbb{R}^2$. Then, we have $X = \mathbb{R}^2 \times \{0\}^{\phi(n)-2}$ and $Y = \{0\}^2 \times \mathbb{R}^{\phi(n)-2}$, where ϕ denotes Euler's totient function; see [7], and [AO1, Secs. 3.4 and 7.3] for more details including the specification of the corresponding lattice in $\mathbb{R}^{\phi(n)}$.

Since $D_X = \mathcal{O}_n$, we are looking at one-dimensional X-rays parallel to $\mathcal{O}_n$-lines. In this context, [25] gave a general characterisation of when exactly the index of the corresponding Siegel grid is finite. As a particular

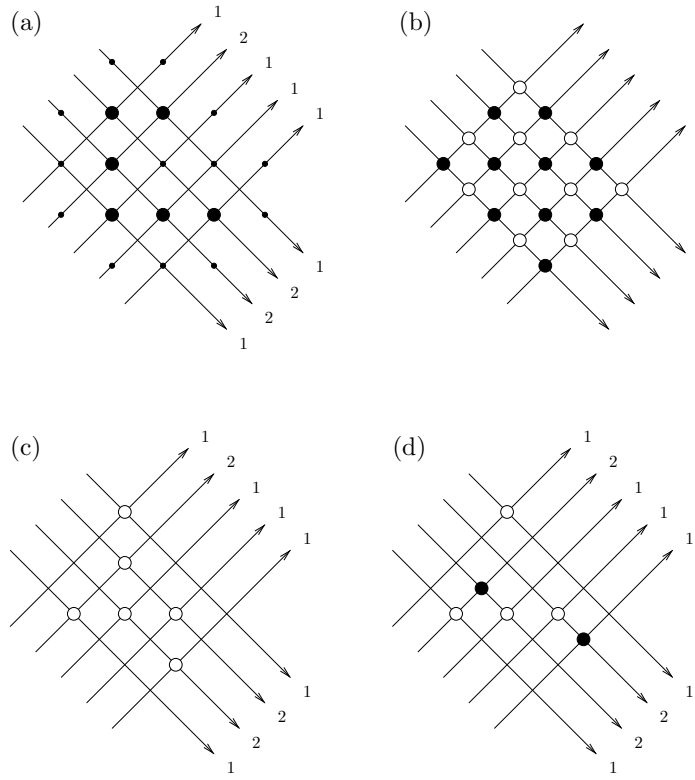

FIGURE 2.5.1. (a) The X-ray lines parallel to $S_1 = \mathrm{lin}\big(\{(1,1)^T\}\big)$ and $S_2 = \mathrm{lin}\big(\{(1,-1)^T\}\big)$ that hit a subset F of $\mathbb{Z}^2$, thus defining an instance $\mathcal{I}$ of $\textsc{Consistency}_{\mathcal{F}^2}(S_1, S_2)$. (b) The grid G falls into two translates of $\mathbb{Z}^2$ (black and white). (c) A set F' with the same X-rays as F contained in the 'white' translate. (d) Another set F'' with the same X-rays scattered over both translates, hence F'' is not a solution to $\mathcal{I}$.

consequence of this characterisation, it is shown in [25] that, in each planar model set whose underlying dimension d is odd, there must exist two module lines whose complete tomographic grid fails to decompose into finitely many equivalence classes.

2.5.3. The separation problem

While the window W may be quite general for non-algorithmic issues, we will assume for the purpose of this section that W is bounded and open (this is the *generic* case; see [7] for a discussion), and that W is given through finitely many linear inequalities, hence W is an open *polytope*. More precisely,

the latter means that W is of the form $\{y \in Y \mid c_i^T y < \beta_i \text{ for } i \in [p]\}$ for some $p \in \mathbb{N}$, $c_i \in Y$ and $\beta_i \in \mathbb{R}$.

Of course, when dealing with model sets, any solution F_X of a given instance of the reconstruction problem must satisfy the additional constraint that $F_X^\star$ is contained in a translate of W. This is the geometric *separation problem* introduced in [6, 7].

As it turns out, there is no simple way around the obvious problems of working in the binary Turing machine model. In fact, if we lift the problem again into $\mathbb{R}^d$, not even the basic task to check whether a vector $z \in \mathbb{Z}^d$ satisfies the constraints $c^T z < \beta$ can be performed in finite precision if the normal c is not rational. However, in terms of the number of arithmetic operations over the reals, the problem is easy.

2.5.4. Results for the real RAM model

In the following, we apply the real RAM model of computation where each of the standard elementary operations on the reals counts only with unit cost. Using results from [14] on the computation of hyperplane arrangements, [7] shows that, in the real RAM model, the separation problem can indeed be solved efficiently.

Theorem 2.5.1 ([7]). *For any finite subset $F \subset \mathbb{R}^d$, the separation problem can be solved in $O\big(\mathrm{card}(F)^{d+1}\big)$ real operations.* □

Since [7] also shows that the decomposition problem for cyclotomic model sets can be solved in polynomial time in the real RAM model, it follows that the standard tomographic algorithms that have been developed for the lattice case can be extended to cyclotomic model sets. Hence, one can solve the consistency, reconstruction and uniqueness problem for two X-rays efficiently. For convenience, let us formulate the problem $\textsc{Consistency}_{\mathcal{F}}(S_1, S_2)$ more precisely. The other two tasks are defined analogously.

Let again $X = \mathbb{R}^2 \times \{0\}^{\phi(n)-2}$, $Y = \{0\}^2 \times \mathbb{R}^{\phi(n)-2}$, let W be an open polytope in Y, and set

$$\mathcal{F} = \{F \mid F \subset \mathcal{O}_n \text{ finite}, \exists M \in \mathcal{M}(W) : F^\star \subset M\}.$$

Further, let S_1, S_2 be distinct $\mathcal{O}_n$-lines. Note that this complies with our previous setting since, for any n-cyclotomic model set $\varLambda$, the $\varLambda$-lines are precisely the $\mathcal{O}_n$-lines. Then, we are confronted with the following problem.

$\textsc{Consistency}_{\mathcal{F}}(S_1, S_2)$.
Instance: *Data functions f_1, f_2.*
Question: *Is there an $F \in \mathcal{F}$ such that $X_{S_i}(F) = f_i$ for $i \in \{1, 2\}$?*

Using the results on the decomposition and the separation problem, we obtain the following result.

Theorem 2.5.2 ([7]). *Consistency$_{\mathcal{F}}(S_1, S_2)$, Reconstruction$_{\mathcal{F}}(S_1, S_2)$ and Uniqueness$_{\mathcal{F}}(S_1, S_2)$ can be solved with polynomially many operations and polynomially many calls to an oracle that solves the same problem on subsets of the plane of cardinality $O(q^2)$, where q is the maximum of the cardinalities of the supports of the given X-ray data functions.* □

As a simple corollary to Theorems 2.4.1 and 2.5.2, we see that the case of two lines can be solved in polynomial time even for cyclotomic model sets.

Corollary 2.5.3 ([7]). *Consistency$_{\mathcal{F}}(S_1, S_2)$, Reconstruction$_{\mathcal{F}}(S_1, S_2)$ and Uniqueness$_{\mathcal{F}}(S_1, S_2)$ can be solved in polynomial time in the real RAM model.* □

2.6. Uniqueness in discrete tomography

From now on, we focus on conditions which guarantee that a given set is uniquely determined by certain of its X-rays. Of course, given the intractability results of Section 2.4, one cannot expect to find general criteria for uniqueness that can be checked efficiently. We will first give some elementary results and then outline generalisations of the uniqueness results of [16] for convex lattice sets under line X-rays to the case of Delone sets.

Recall that a Delone set in $\mathbb{R}^d$ is a uniformly discrete and relatively dense subset of $\mathbb{R}^d$; see [AO1, Def. 2.1]. Throughout this section, we are concerned with a *fixed* Delone set $\varLambda \subset \mathbb{R}^d$. Further, let

$$S_1, \ldots, S_m \in \mathcal{S}_{1,d}(\varLambda)$$

be $\varLambda$-lines; we will consider one-dimensional X-rays parallel to these given lines. For a collection $\mathcal{E} \subset \mathcal{F}(\varLambda, \{0,1\})$ of finite subsets of $\varLambda$, we ask whether there are different *tomographically equivalent* sets $F, F' \in \mathcal{E}$, which means that

$$X_{S_i} F = X_{S_i} F' \quad \text{for all } i \in [m].$$

If this is not the case, we say that the elements of $\mathcal{E}$ are *determined* by the X-rays parallel to $S_1, \ldots, S_m$. In this situation, any element F of $\mathcal{E}$ can be distinguished from any other element of $\mathcal{E}$ just by looking at its X-rays parallel to $S_1, \ldots, S_m$.

2.6.1. Elementary uniqueness results for general Delone sets

If one allows for arbitrary finite subsets of $\varLambda$ and starts from any given finite set of $\varLambda$-lines, one can, under relatively mild assumptions (which are satisfied by many model sets), construct two different finite subsets of $\varLambda$ with

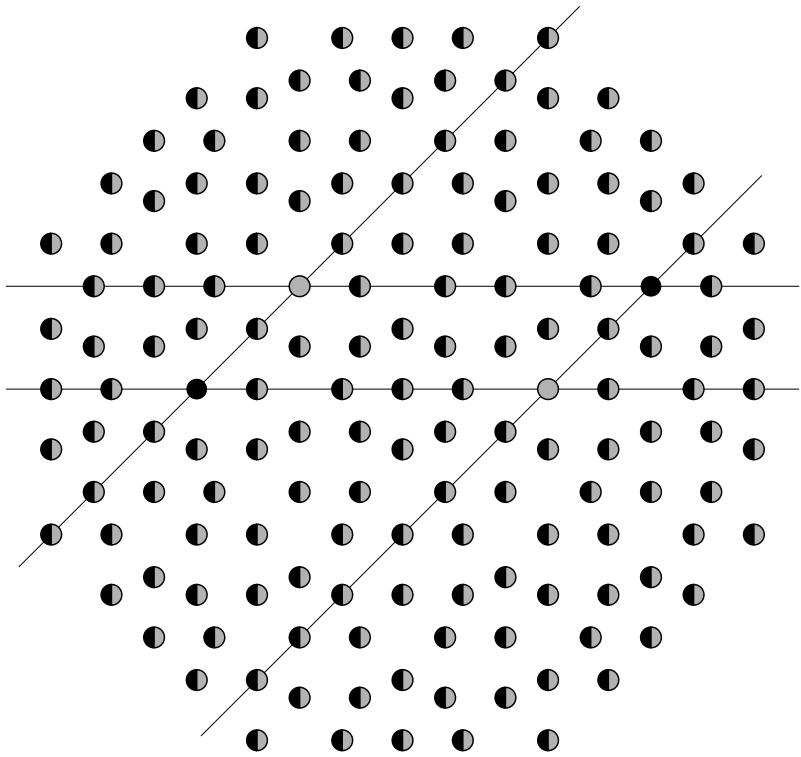

FIGURE 2.6.1. Two subsets (black versus grey) of a finite patch of a Delone set $\varLambda$ which have the same X-rays parallel to the two indicated $\varLambda$-lines. The half-split (black and grey) points belong to both sets.

the same X-rays parallel to these lines. A typical situation is illustrated in Figure 2.6.1.

For instance, this situation occurs if any finite subset of the Abelian group generated by the difference set $\varLambda - \varLambda$ maps, under a suitable homothety of $\mathbb{R}^d$, into the point set $\varLambda$ itself. Note that any translate $t + L$ of a lattice L trivially has this property, since $L - L = L$. Another important class of planar examples is given by *algebraic Delone sets*; see Definition 2.6.3 below.

The first general uniqueness result is due to [45] and holds for arbitrary point sets in $\mathbb{R}^d$; see also [17, Thm. 4.3.3]. The following formulation is specialised to our Delone set $\varLambda$ at hand.

Proposition 2.6.1 ([45])**.** *The finite subsets F of $\varLambda$ with* $\mathrm{card}(F) \leqslant k$ *are determined by the X-rays parallel to any set of $k+1$ or more $\varLambda$-lines. In fact, these sets then coincide with their associated grids.* □

In real world applications, the atomic structures to be determined comprise about 10^6 to 10^9 atoms. This unfortunately implies that Proposition 2.6.1 is not practical at all.

Another possibility for obtaining positive uniqueness results is the systematic use of $\varLambda$-lines that yield sparsely occupied lines in $\varLambda$. To be more specific, recall that a Delone set $\varLambda$ is said to be of *finite local complexity* (FLC) if, for every $r > 0$, there are only finitely many *patches of radius* r up to translations. Here, a patch refers to a set of the form $\varLambda \cap B_r(x)$ with $x \in \mathbb{R}^d$; see [AO1, Ch. 2] for background information. In particular, a Delone set $\varLambda$ is FLC if and only if $\varLambda - \varLambda$ is locally finite. One has the following result.

Proposition 2.6.2 ([35, Prop. 3.5])**.** *Let $\varLambda$ be an FLC Delone set and fix some $r > 0$. The subsets of patches of radius r of $\varLambda$ are determined by the X-rays parallel to a suitable set of two $\varLambda$-lines. Moreover, with respect to a suitable set of three $\varLambda$-lines, each such set coincides with its associated grid.* □

Note that such lines, in a sense, approximate the illegitimate non-$\varLambda$-lines. For precisely this reason, they are also rather useless in practice. In contrast, experimentally accessible is only the situation with spatially well-separated lines of high occupation; see [44] and references therein for an analysis of this geometric situation.

2.6.2. Uniqueness results for algebraic Delone sets

The results of Propositions 2.6.1 and 2.6.2 either require an inappropriately large number of X-rays or X-ray-lines whose intersection with $\varLambda$ is so sparse that they do not lead to a suitable (experimental) resolution. These results are, nevertheless, the only presently available uniqueness results for general subsets of $\varLambda$.

In what follows, we thus derive a uniqueness result for a more restricted class of planar Delone sets. To this end, we generalise the notion of convex lattice sets from Section 2.4.1. A subset F of $\varLambda$ is called *convex* if

$$F \,=\, \mathrm{conv}(F) \cap \varLambda.$$

In the sequel, we consider convex subsets of such Delone sets in the Euclidean plane which, when seen as subsets of the complex numbers, satisfy strong algebraic properties and are therefore called *algebraic* Delone sets; see Definition 2.6.3 below. These sets form a rich class that contains all conventional structure models for planar quasicrystals with non-trivial rotational symmetry, the latter appearing as typical slices of quasicrystals in nature.

Let us make the formulation in terms of complex numbers more precise; compare [AO1, Sec. 3.4.2] for background. The complex conjugate of a complex number $z \in \mathbb{C}$ is denoted by $\bar{z}$, and $|z| = \sqrt{z\bar{z}}$ is its modulus. Recall that an $\mathbb{R}$-linear endomorphism (resp., affine endomorphism) ψ of $\mathbb{C}$ is given by $z \mapsto az + b\bar{z}$ (resp., $z \mapsto az + b\bar{z} + t$), where $a, b, t \in \mathbb{C}$. In both cases, ψ is an automorphism if and only if $\det(\psi) = a\bar{a} - b\bar{b} \neq 0$. A *homothety* ψ of $\mathbb{C}$ is an affine automorphism given by $z \mapsto \lambda z + t$, where $\lambda > 0$ and $t \in \mathbb{C}$.

Now, we denote by $K_{\varLambda}$ the intermediate field of $\mathbb{C}/\mathbb{Q}$ that is given by

$$K_{\varLambda} \,=\, \mathbb{Q}\big((\varLambda - \varLambda) \cup \big(\overline{\varLambda - \varLambda}\,\big)\big)\,, \tag{2.6.1}$$

the latter being the smallest subfield of $\mathbb{C}$ that contains both $\varLambda - \varLambda$ and its image $\overline{\varLambda - \varLambda}$ under complex conjugation. For $n \in \mathbb{N}$, we set $\zeta_n = \mathrm{e}^{2\pi\mathrm{i}/n}$, a primitive nth root of unity. Then, $\mathbb{Q}(\zeta_n)$ is the nth cyclotomic field, with

$$[\mathbb{Q}(\zeta_n) : \mathbb{Q}] \,=\, \phi(n).$$

Note that $\mathbb{Q}(\zeta_n) = \mathbb{Q}(\zeta_N)$, where here and below $N = N(n) = \mathrm{lcm}(n, 2)$.

Definition 2.6.3. A Delone set $\varLambda \subset \mathbb{C}$ is called an *algebraic Delone set* if $K_{\varLambda}$ from Eq. (2.6.1) is an algebraic number field (i.e., $[K_{\varLambda} : \mathbb{Q}] < \infty$) and if any finite subset of $K_{\varLambda}$ maps into $\varLambda$ under a suitable homothety of the complex plane. An algebraic Delone set $\varLambda$ is called an *n-cyclotomic Delone set* if it satisfies $K_{\varLambda} \subseteq \mathbb{Q}(\zeta_n)$ with $n \geqslant 3$. Further, $\varLambda$ is called a *cyclotomic Delone set* if it is an n-cyclotomic Delone set for some $n \geqslant 3$.

Let us point out that, for every algebraic Delone set $\varLambda$, the field extension $K_{\varLambda}/\mathbb{Q}$ is an imaginary extension (due to the relative denseness of $\varLambda$) with $\overline{K_{\varLambda}} = K_{\varLambda}$. Using standard Minkowski theory from algebraic number theory together with results from the theory of Pisot–Vijayaraghavan (PV) numbers, compare [AO1, Def. 2.13], it was shown in [36] that, for every imaginary quadratic extension K of a real algebraic number field, one can construct algebraic Delone sets $\varLambda$ with $K_{\varLambda} = K$. In fact, these examples are model sets, the so-called *K-algebraic model sets*.

The most important examples of this type are the *n-cyclotomic model sets* $\varLambda$, where $K_{\varLambda} = \mathbb{Q}(\zeta_n)$; see [AO1, Sec. 7.3] for details. For suitably chosen windows, these sets have N-fold rotational symmetry. For instance, Figure 2.6.1 above shows a central patch of vertices of the eightfold *Ammann–Beenker tiling*; compare [5] and see [AO1, Ex. 7.8 and Fig. 7.4] for its description as an 8-cyclotomic model set. As another example, Figure 2.6.2 on page 63 below shows a central patch of Gähler's twelvefold *shield tiling*, a 12-cyclotomic model set; see [22] and [AO1, Ex. 7.12].

Generalising results of [16] for convex lattice sets, we will now show that the convex subsets of an algebraic Delone set $\varLambda$ can be determined by the X-rays either in four suitably chosen or in any sufficiently large finite collection

of $\varLambda$-lines, where the required number of $\varLambda$-lines only depends on $\varLambda$. In fact, the notion of an algebraic Delone set is tailor-made such that the approach from [16] allows for such a generalisation. In particular, it turns out that the uniqueness problem can be reformulated in terms of the non-existence of certain polygons.

For a point set $X \subset \mathbb{R}^2$, a *polygon* in X is the convex hull of finitely many points of X. As in the lattice case [20, 16], particular polygons play a decisive role in the uniqueness theorem, namely those whose vertices correspond to the components of the symmetric difference of two tomographically equivalent subsets F and F' of $\mathbb{R}^2$. Before we define them, note that, in general, if two finite subsets F and F' of $\mathbb{R}^d$ have the same X-rays parallel to some line S, one not only has $\operatorname{card}(F) = \operatorname{card}(F')$, but also that the *centroids* (or barycentres) of F and F' lie on the same line parallel to S. Thus, the centroids of F and F' coincide if F and F' have the same X-rays parallel to two or more lines.

Definition 2.6.4. Let U be a finite set of lines through the origin in the plane. A non-degenerate convex polygon P is called a *U-polygon* if it has the property that, whenever v is a vertex of P and $S \in U$, the line $v + S$ also meets another vertex v' of P.

By a *regular polygon* we shall always mean a non-degenerate convex regular polygon. An *affinely regular polygon* is the image of a regular polygon under an affine automorphism of the plane. Clearly, U-polygons have an even number of vertices. Moreover, an affinely regular polygon with an even number of vertices is a U-polygon if and only if each line from U is parallel to one of its edges.

The following result exhibits the geometric content of tomographical equivalence. It was proved in [16] for the lattice case and later extended to algebraic Delone sets in [34]. Note that the proof of implication (ii) $\Longrightarrow$ (i) and the additional statement only require the homothety property of algebraic Delone sets. The finiteness of the dimension of $K_{\varLambda}$ as a vector space over $\mathbb{Q}$ will play a crucial role later on.

Theorem 2.6.5. *Let $\varLambda$ be an algebraic Delone set and let U be a set of two or more $\varLambda$-lines. Then, the following statements are equivalent.*

(i) *The convex subsets of $\varLambda$ are determined by the X-rays parallel to the lines from U.*

(ii) *There is no U-polygon in $\varLambda$.*

In addition, for $\operatorname{card}(U) \leqslant 3$*, there always is a U-polygon in $\varLambda$.*

Sketch of proof. To show (i) $\Longrightarrow$ (ii), suppose the existence of a U-polygon P in $\varLambda$. Partition the vertices of P into two disjoint sets V and V', where the elements of these sets alternate along the boundary ∂P of P.

Since P is a U-polygon, each line in the plane parallel to some $S \in U$ that contains a point in V also contains a point in V'. Set $C = (\varLambda \cap P) \setminus (V \cup V')$. Then, $F = C \cup V$ and $F' = C \cup V'$ are different convex subsets of $\varLambda$ with the same X-rays parallel to the lines from U; see Figure 2.6.2 for an illustration.

Now, for the implication (ii) $\Longrightarrow$ (i), suppose that F and F' are different convex subsets of $\varLambda$ with the same X-rays parallel to the lines from U. In particular, $\mathrm{card}(F) = \mathrm{card}(F')$ and F and F' have the same centroid. By the additional statement proved below, we may assume that $\mathrm{card}(U) \geqslant 4$. Without restriction, we may further assume that $0 \in \varLambda$, whence all rational linear combinations of elements from $\varLambda$ (like centroids of finite subsets of $\varLambda$) belong to $K_\varLambda$. The set $E = \mathrm{conv}(F) \cap \mathrm{conv}(F')$ has non-empty interior, since the common centroid of F and F' is in fact an interior point of E.

Clearly, the symmetric difference $\mathrm{conv}(F) \triangle \mathrm{conv}(F')$ has only finitely many connected components. Due to $F \neq F'$, there is at least one component, C say. Then, $C \cap \varLambda$ consists of points of F or F' only and, for any line $S \in U$, it follows from the identity $X_S F = X_S F'$ that there is another component C_S (on the 'opposite side') such that $X_S(C \cap \varLambda) = X_S(C_S \cap \varLambda)$. Then, the centroids of $C \cap \varLambda$ and $C_S \cap \varLambda$ lie on the same line parallel to S. One can now verify that a suitable collection of points from the finite set of centroids of sets of the form $C \cap \varLambda$, where C is a component of $\mathrm{conv}(F) \triangle \mathrm{conv}(F')$, form the vertices of a U-polygon in $K_\varLambda$. Applying a suitable homothety finally yields a U-polygon in $\varLambda$.

Finally, for the additional claim, we may assume that $\mathrm{card}(U) = 3$. First, construct a triangle in $K_\varLambda$ having sides parallel to the given lines from U. If two of the vertices are chosen in $K_\varLambda$, then the third is automatically in $K_\varLambda$. Now, assemble six congruent versions of this triangle in the obvious way to make an affinely regular hexagon in $K_\varLambda$. The latter is then a U-polygon in $K_\varLambda$ and applying a suitable homothety gives the desired U-polygon in $\varLambda$. □

Example 2.6.6. Let $\varLambda$ be an algebraic Delone set with $K_\varLambda = \mathbb{Q}(\zeta_n)$ for some $n \geqslant 3$, a so-called *strongly* (*or fully*) *n-cyclotomic Delone set*. Note that n-cyclotomic model sets are of this type. Consider the regular N-gon $R \subset \mathbb{Q}(\zeta_n)$ inscribed in the unit circle, with one vertex at 1. Attach now N translates of R edge-to-edge to R in the obvious way (which generally overlap). Then, one can easily verify that the convex hull P of the resulting point set is a U-polygon in $\mathbb{Q}(\zeta_n)$, where U is the set of N distinct lines from $\mathcal{S}_{1,2}(\mathbb{Q}(\zeta_n))$ given by the edges and diagonals of R. Employing a suitable homothety gives a U-polygon in $\varLambda$ and one sees that U actually consists of N distinct $\varLambda$-lines; see Figure 2.6.2 for an illustration of the construction (the grey lines indicate the $N = 12$ translates of R). For the two crystallographic cases $n = 3$ and $n = 4$, the corresponding cyclotomic fields are linearly equivalent. It is thus clear that, as it is the case for the triangular lattice,

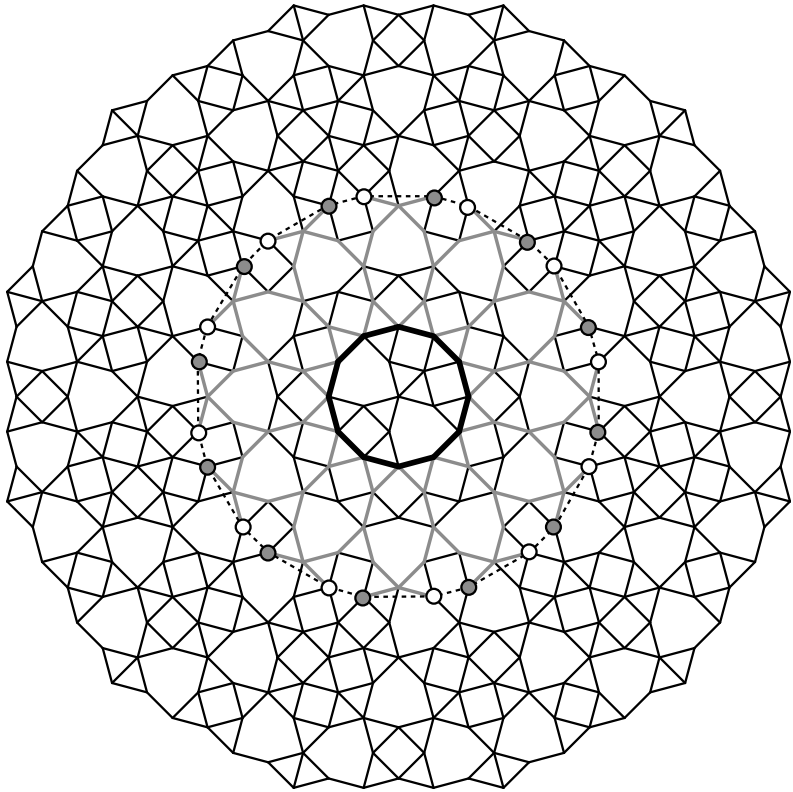

FIGURE 2.6.2. A U-polygon (its boundary being indicated by the dotted line) in the vertex set Λ of the twelvefold shield tiling, where U is the set of $N = 12$ Λ-lines given by the edges and diagonals of the central regular dodecagon (its boundary being indicated by the bold line). The vertices of Λ in the interior of the U-polygon together with the vertices indicated by the white or the grey dots, respectively, give two different convex subsets of Λ with the same X-rays in the directions of U.

also the square lattice contains a U-polygon for a set U consisting of *six* (and not only $N = 4$) Λ-lines; compare [16, Fig. 1] and [17, Fig. 4.5]. $\Diamond$

The above example in conjunction with Theorem 2.6.5 immediately implies the following lower bound on the so-called *magic number* c_Λ. We will demonstrate in Theorem 2.6.11 that these magic numbers are always finite, and we will provide a formula for the smallest possible magic numbers in certain cases.

Proposition 2.6.7. *Let Λ be a strongly n-cyclotomic Delone set. Then, the smallest possible number c_Λ with the property that any two convex subsets of*

$\varLambda$ can be distinguished by the X-rays in any set of $c_{\varLambda}$ $\varLambda$-lines satisfies $c_{\varLambda} \geqslant 7$ for $n = 4$ and

$$c_{\varLambda} \geqslant N + 1$$

for all other values of $n \geqslant 3$, with $N = \mathrm{lcm}(n, 2)$. □

Remark 2.6.8. The number 7 in Proposition 2.6.7 can be seen as a special case of the general lower bound as follows. Clearly, the crystallographic cases $n = 3$ and $n = 4$ are equivalent via an affine transformation. While the traditional formulation uses the square lattice, hence $n = 4$, one could equally well work with the triangular lattice, where $n = 3$ means $N = 6$, which gives $N + 1 = 7$. ◊

The proof of the following central result uses Darboux's theorem on second midpoint polygons which states that, given any convex polygon with centroid at the origin, the sequence of successive second midpoint polygons converges, when dilated in each step to keep the area constant, to an affinely regular polygon; see [13] as well as [15, Ch. 1] or [20].

Proposition 2.6.9 ([15, 20])**.** *Let U be a finite set of one-dimensional subspaces of the Euclidean plane. Then, there exists a U-polygon if and only if there is an affinely regular polygon such that each line in U is parallel to one of its edges.* □

Note that a U-polygon need not be affinely regular, even if it is a U-polygon in a cyclotomic model set. For example, there is a U-icosagon in the vertex set of the *Tübingen triangle tiling* of the plane (a 5-cyclotomic model set; see [8, AO1] and [34, Fig. 1, Cor. 14 and Ex. 15]), which cannot be affinely regular since that restricts the number of vertices to 3, 4, 5, 6 or 10 by [32, Cor. 4.2]; see also [16, Ex. 4.3] for an example in the case of the square lattice. In general, there is an affinely regular polygon with $n \geqslant 3$ vertices in an algebraic Delone set $\varLambda$ if and only if $\mathbb{Q}(\zeta_n) \cap \mathbb{R} \subset K_{\varLambda} \cap \mathbb{R}$, the latter being a relation that (due to $[K_{\varLambda} : \mathbb{Q}] < \infty$) can only hold for finitely many values of n; compare [32, Thm. 3.3]. This also shows that the U-polygon with 24 vertices shown in Figure 2.6.2 cannot be affinely regular.

Let (t_1, t_2, t_3, t_4) be an ordered tuple of four distinct elements of $\mathbb{R} \cup \{\infty\}$. Then, its *cross-ratio* $\langle t_1, t_2, t_3, t_4 \rangle$ is the non-zero real number defined by

$$\langle t_1, t_2, t_3, t_4 \rangle = \frac{(t_3 - t_1)(t_4 - t_2)}{(t_3 - t_2)(t_4 - t_1)}, \tag{2.6.2}$$

with the usual conventions if one of the t_i equals ∞.

Remark 2.6.10. The cross-ratio of slopes of distinct lines S_1, S_2, S_3, S_4 through the origin is invariant under $\mathbb{R}$-linear automorphisms of the complex plane. ◊

We can now state our main result on U-polygons which is an extension of [16, Thm. 4.5] due to [35, 36]. The finiteness assertions rely on the finiteness of the degree of K_Λ over $\mathbb{Q}$.

Theorem 2.6.11. *Let Λ be an algebraic Delone set. Further, let U be a set of four or more Λ-lines and suppose the existence of a U-polygon. Then, the cross-ratio of slopes of any four lines from U, arranged in order of increasing angle with the positive real axis, is a number in the field $K_\Lambda \cap \mathbb{R}$ that can be written in the form*

$$\frac{\bigl(1-\zeta_m^{k_1}\bigr)\bigl(1-\zeta_m^{k_2}\bigr)}{\bigl(1-\zeta_m^{k_3}\bigr)\bigl(1-\zeta_m^{k_4}\bigr)},$$

where $(k_1,k_2,k_3,k_4) \in \mathbb{N}^4$ satisfies $k_3 < k_1 \leqslant k_2 < k_4 \leqslant m-1$ together with $k_1+k_2 = k_3+k_4$. Moreover, there are only finitely many such numbers and $\mathrm{card}(U)$ *is bounded from above by a finite number $b_\Lambda \in \mathbb{N}$ that only depends on Λ.*

Sketch of proof. Let U be as in the assertion. One calculates that the slope of each line in U is contained in $(K_\Lambda \cap \mathbb{R}) \cup \{\infty\}$. Thus, the cross-ratio of slopes of any four lines from U is a number in the field $K_\Lambda \cap \mathbb{R}$. By Proposition 2.6.9, U consists of lines parallel to the edges of an affinely regular polygon. There is thus a linear automorphism ψ of the complex plane such that

$$V \,=\, \bigl\{\psi(S) \mid S \in U\bigr\}$$

is contained in a set of equiangular lines through the origin, meaning that the angle between each pair of adjacent lines is the same. Since the lines from U are distinct, we may assume that there is an $m \geqslant 4$ such that each line from V is parallel to a direction that can be represented by a complex number of the form $\mathrm{e}^{h\pi\mathrm{i}/m}$, where $h \in \mathbb{N}_0$ satisfies $h \leqslant m-1$. Let S_j, with $1 \leqslant j \leqslant 4$, be four lines from U, arranged in order of increasing angle with the positive real axis, say $\mathrm{e}^{h_j\pi\mathrm{i}/m} \in \psi(S_j)$, where we may assume that the h_j increase with j. By Remark 2.6.10, the cross-ratio q of slopes of these four lines, in order of increasing angle with the positive real axis, is

$$\begin{aligned} q \,&=\, \frac{\bigl(\tan\bigl(\frac{h_3\pi}{m}\bigr)-\tan\bigl(\frac{h_1\pi}{m}\bigr)\bigr)\bigl(\tan\bigl(\frac{h_4\pi}{m}\bigr)-\tan\bigl(\frac{h_2\pi}{m}\bigr)\bigr)}{\bigl(\tan\bigl(\frac{h_3\pi}{m}\bigr)-\tan\bigl(\frac{h_2\pi}{m}\bigr)\bigr)\bigl(\tan\bigl(\frac{h_4\pi}{m}\bigr)-\tan\bigl(\frac{h_1\pi}{m}\bigr)\bigr)} \\ &=\, \frac{\sin\bigl(\frac{(h_3-h_1)\pi}{m}\bigr)\sin\bigl(\frac{(h_4-h_2)\pi}{m}\bigr)}{\sin\bigl(\frac{(h_3-h_2)\pi}{m}\bigr)\sin\bigl(\frac{(h_4-h_1)\pi}{m}\bigr)}. \end{aligned}$$

Setting $k_1 = h_3-h_1$, $k_2 = h_4-h_2$, $k_3 = h_3-h_2$ and $k_4 = h_4-h_1$, one gets $1 \leqslant k_3 < k_1, k_2 < k_4 \leqslant m-1$ and $k_1+k_2 = k_3+k_4$. Using

$\sin(\theta) = \frac{\mathrm{i}}{2}\,\mathrm{e}^{-\mathrm{i}\theta}(1-\mathrm{e}^{2\mathrm{i}\theta})$, one finally obtains

$$K_{\varLambda} \cap \mathbb{R} \ni q = \frac{\bigl(1-\zeta_m^{k_1}\bigr)\bigl(1-\zeta_m^{k_2}\bigr)}{\bigl(1-\zeta_m^{k_3}\bigr)\bigl(1-\zeta_m^{k_4}\bigr)}. \tag{2.6.3}$$

If necessary, the first two coordinates are interchanged to ensure that $k_1 \leqslant k_2$. This proves the first assertion.

Clearly, in order to prove the second assertion, one has to study the possible solutions of Eq. (2.6.3). Note that q will always be greater than one. For $q \in \mathbb{Q}$, this has been done in [16] by employing the powerful tool of p-adic valuations; see [17] for a gentle description of the method. It turns out that, for $q = 2$, there are infinite families of solutions of the type

$$\frac{\bigl(1-\zeta_m^{2k}\bigr)\bigl(1-\zeta_m^{s}\bigr)}{\bigl(1-\zeta_m^{k}\bigr)\bigl(1-\zeta_m^{k+s}\bigr)} = 2, \tag{2.6.4}$$

where $s \geqslant 2$, $m = 2s$ and $1 \leqslant k \leqslant \frac{s}{2}$ (or $\frac{s}{2} \leqslant k < s$ if the two factors in the numerator are interchanged). Apart from these infinite families, there are only finitely many 'sporadic' solutions (up to multiplication of m and (k_1, k_2, k_3, k_4) by the same factor), all of which can be written with $m = 12$. For example, one has

$$\frac{\bigl(1-\zeta_6^{2}\bigr)\bigl(1-\zeta_6^{2}\bigr)}{\bigl(1-\zeta_6^{1}\bigr)\bigl(1-\zeta_6^{3}\bigr)} = \frac{\bigl(1-\zeta_{12}^{4}\bigr)\bigl(1-\zeta_{12}^{4}\bigr)}{\bigl(1-\zeta_{12}^{2}\bigr)\bigl(1-\zeta_{12}^{6}\bigr)} = \frac{3}{2}.$$

In fact, the possible rational values of q that occur among the solutions are $\frac{4}{3}$, $\frac{3}{2}$, 2, 3 and 4.

The solutions with irrational values of q (i.e., $q \in (K_{\varLambda} \cap \mathbb{R}) \setminus \mathbb{Q}$) can now be treated by standard methods from the theory of cyclotomic fields; see [36] for further details. In fact, this approach works for all values of $q \in K_{\varLambda} \cap \mathbb{R}$ except the special value $q = 2$ that leads to the infinite families described above. From the perspective of this approach, the special role of $q = 2$ is the property that it is the unique real number greater than one that can be written in the form $\frac{1+x}{1+y}$, where x as well as y is either a root of unity in $\mathbb{C}$ or equal to zero [36, Lemma 4.4]. Using the finiteness of the degree of $K_{\varLambda}$ over $\mathbb{Q}$, one can show that no new infinite families but only finitely many further 'sporadic' solutions do occur, all of which can be written with a common finite value $m = m_{\varLambda}$; see [36, Thm. 4.9]. In particular, this shows that only finitely many values of q occur in the solutions.

It remains to show the boundedness of $\mathrm{card}(U)$. Suppose $\mathrm{card}(U) \geqslant 7$, let U' consist of seven lines from U and let

$$V' = \bigl\{\psi(S) \mid S \in U'\bigr\}.$$

Clearly, one of the first two quadrants, say the first, meets at least four lines from V'. An application of the above argument to some four of these lines

gives integers h_j satisfying $0 \leqslant h_1 < h_2 < h_3 < h_4 \leqslant \frac{m}{2}$, where we may also assume, by rotating the lines from V' if necessary, that $h_1 = 0$. As above, we obtain a corresponding solution of Eq. (2.6.3). This solution cannot be of the form (2.6.4) since, using $h_1 = 0$, one obtains $h_4 = k_4 = k + s > \frac{m}{2}$, a contradiction. Thus, our solution must correspond to one of the finitely many 'sporadic' solutions with $m = m_{\varLambda}$. One can see that each line from U corresponds to an angle with the positive real axis which is an integer multiple of $\pi/m_{\varLambda}$ and thus corresponds to an integer h in the set $\{0, 1, \ldots, m_{\varLambda} - 1\}$. This shows that $\mathrm{card}(U)$ is bounded. □

As a consequence, we obtain our main result on the determination of convex subsets of algebraic Delone sets.

Theorem 2.6.12. *Let $\varLambda$ be an algebraic Delone set.*

(a) *There are sets of four $\varLambda$-lines such that the convex subsets of $\varLambda$ are determined by the corresponding X-rays. In addition, less than four $\varLambda$-lines never suffice for this purpose.*

(b) *There is a finite number $c_{\varLambda} \in \mathbb{N}$ such that the convex subsets of $\varLambda$ are determined by the X-rays parallel to any set of $c_{\varLambda}$ distinct $\varLambda$-lines.*

Proof. To prove (a), it suffices, by Theorems 2.6.5 and 2.6.11, to take any set of four $\varLambda$-lines such that the cross-ratio of their slopes, arranged in order of increasing angle with the positive real axis, is not an element of a certain finite subset of $K_{\varLambda} \cap \mathbb{R}$. Since there are infinitely many $\varLambda$-lines, one may fix three $\varLambda$-lines and let the fourth one vary in order to see that the set of cross-ratios of slopes of four $\varLambda$-lines, arranged in order of increasing angle with the positive real axis, is infinite as well. This establishes the assertion. The additional statement follows immediately from the additional statement of Theorem 2.6.5. Part (b) is also a direct consequence of Theorems 2.6.5 and 2.6.11. □

A list of cross-ratios to be avoided in the practically most important cases $n = 5, 8$ and 12 of quasicrystallography can be found in [36, Cor. 4.10] and [37].

A major step in the proof of Theorem 2.6.11 is the treatment of the special case of n-cyclotomic Delone sets $\varLambda$. Here, it turns out that the 'sporadic' solutions of Eq. (2.6.3) can be written with $m_{\varLambda} = \mathrm{lcm}(2n, 12)$. Moreover, for strongly n-cyclotomic Delone sets $\varLambda$, one can show by direct computation that, with the exception of $b_4 = 6$, for $3 \leqslant n \leqslant 50$, the trivial lower bound $b_n = N$ (compare Example 2.6.6) is in fact an upper bound for the cardinality of sets U of $\varLambda$-lines that allow U-polygons. In addition, for these values of n, if there is a U-polygon with $\mathrm{card}(U) = N$, then there is a linear automorphism

of the plane that takes the lines from U to a set of lines which are represented by $\mathrm{e}^{h\pi\mathrm{i}/N}$, where $h \in \{0, 1, 2, \ldots, N-1\}$; see [37, Thm. 2] and Figure 2.6.2. We conjecture that $b_n = N$ (with the exception of $b_4 = 6$) is indeed the best possible upper bound for the cardinalities of sets U of $\varLambda$-lines that allow U-polygons for *all* values of $n \geqslant 3$.

Hence, for strongly n-cyclotomic Delone sets $\varLambda$ with $3 \leqslant n \leqslant 50$, with the exception of $c_4 = 7$, the convex subsets of $\varLambda$ are determined by the X-rays parallel to any set of $c_n = N + 1$ $\varLambda$-lines. This leads to the following open problem in the DT of strongly cyclotomic Delone sets.

Conjecture 2.6.13. *For $n \geqslant 3$, the smallest possible magic numbers c_n for strongly n-cyclotomic Delone sets are given by $c_4 = 7$ and by $c_n = N + 1$ for all other values of n, where $N = \mathrm{lcm}(n, 2)$.*

Let us close with two final comments. Theorem 2.6.12 gives rise to the problem of how to reconstruct a convex subset of an n-cylotomic model set $\varLambda$ from its X-rays in a set of $\varLambda$-lines that guarantee a unique solution. While by [10] this can be done efficiently in the lattice case, this problem is open for more general $\varLambda$.

A slice by slice application of Theorem 2.6.12 immediately gives corresponding results on the determination of convex subsets of typical three-dimensional model sets $\varLambda$ by X-rays parallel to $\varLambda$-lines; compare [33]. These $\varLambda$-lines then clearly lie in a common two-dimensional subspace. It is completely unknown, even in the lattice case, which sets of $\varLambda$-lines in *general position* guarantee uniqueness. There is a long-standing open problem that *seven* might be a universal magic number for the determination of convex subsets of three-dimensional Delone sets $\varLambda$ by X-rays parallel to $\varLambda$-lines in general position. All we know so far is that, if there is such a number, it cannot be smaller than seven; see [15] and [37] for details.

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CHAPTER 3

Geometric Enumeration Problems for Lattices and Embedded $\mathbb{Z}$-Modules

Michael Baake and Peter Zeiner

In this chapter, we want to count and classify certain sublattices of a given lattice, as motivated by crystallography. We use methods from algebra and algebraic number theory to find and enumerate the sublattices according to their index. In addition, we use tools from analytic number theory to determine the asymptotic behaviour of the corresponding counting functions. Our main focus lies on similar sublattices and coincidence site lattices, the latter playing an important role in crystallography. As many results are algebraic in nature, we also generalise them to $\mathbb{Z}$-modules embedded in $\mathbb{R}^d$.

3.1. Introduction

Lattices in $\mathbb{R}^3$ have been used for more than a century in crystallography, as they describe the translational symmetries of idealised, infinitely extended (periodic) crystals. As such, they have been studied intensively, together with space groups, which are finite extensions of lattices (viewed as Abelian groups) and describe the full symmetry of the crystals; compare the Epilogue to this volume. Group-subgroup relations have been applied to analyse various aspects such as phase transitions in crystals.

A special case of the latter is the question of certain kinds of sublattices of a given lattice. Ideal crystals do not exist in nature, and the result of crystallisation is very often not a single crystal, but a mixture of differently orientated crystals of the same kind. The latter are called *grains*, and an important question in crystallography is their mutual orientation and the border between two neighbouring grains, called a *grain boundary*.

To study the latter, one assigns, to each of the two grains, its corresponding lattice, say $\varGamma$ and $\varGamma'$, and computes their intersection $\varGamma \cap \varGamma'$. If the two grains are of the same kind, the two lattices are related by an orthogonal

transformation R, which means that we have $\varGamma' = R\varGamma$ for a suitable isometry $R \in \mathrm{O}(3,\mathbb{R})$. The corresponding sublattice $\varGamma \cap R\varGamma$ is called a *coincidence site lattice* (CSL).

It was Friedel in 1911 who first recognised the usefulness of CSLs in describing and classifying grain boundaries of crystals [37]. Analogous ideas were later used by Kronberg and Wilson [61]. But it still took some time before their ideas became popular. In fact, the widespread use of CSLs was only triggered by a paper of Ranganathan [74] in 1966. Many important papers were published in the following years. In particular, we mention contributions by Grimmer [45, 46, 47, 48, 49, 50] and Bollmann [19, 20].

The discovery of quasicrystals sparked new interest in CSLs, and a systematic mathematical study started. In particular, the concept of CSLs was generalised to $\mathbb{Z}$-modules embedded in $\mathbb{R}^d$, which led to the notion of coincidence site modules (CSMs). They are used to describe grain boundaries in quasicrystals; compare [12, 71, 87] and references therein.

This new development also triggered a more detailed study of lattices in dimensions $d > 3$, as they are used to generate aperiodic point sets by the now common cut and project technique; compare [AO1, Ch. 7]. In particular, lattices in dimension $d = 4$ such as the hypercubic lattices [4, 93] and the A_4-lattice [16, 55] were studied.

Further applications of CSLs can be found in coding theory in connection with so-called lattice quantisers, where lattices in large dimensions and with high packing densities are important; compare [33, 83] for general background, as well as [1] for concrete applications of the A_4-lattice and [2] for the hexagonal lattice. However, not much is known about lattices in dimensions $d > 5$, although there are some partial results for rational lattices; compare [98, 99, 56].

The original concept of CSLs has been generalised in several ways. In particular, one may study the intersection of several rotated copies of a lattice, which are known as multiple CSLs; compare [8, 94, 13]. They have applications to so-called multiple junctions [39, 40, 41], which are multiple crystal grains meeting at some common manifold. Whereas classical CSLs involve only linear isometries, one may consider affine isometries as well, which is directly related to the question of coincidences of crystallographic point packings; compare [63, 65, 62]. The latter are connected to the problem of coincidences of coloured lattices and colour coincidences [64, 62, 66].

The planar case is certainly the best studied. Here, also a connection between CSLs and well-rounded sublattices has been established [18]. Moreover, even some results for the hyperbolic plane [77] have been found.

Naturally, CSLs are not the only sublattices that are of interest in crystallography and coding theory. Classifying sublattices with certain symmetry

constraints has a long tradition in mathematics and in crystallography; compare [78, 79] and references therein. An interesting question is the number of sublattices that are *similar* to its parent lattice. It has been answered in detail for a considerable collection of lattices [7, 11, 15] in dimensions $d \leqslant 4$. For higher dimensions, some existence results have been obtained by Conway, Rains and Sloane, who were motivated by problems in coding theory [25].

Actually, some years ago, a close connection between *similar sublattices* (SSLs) and CSLs has been established [42], which was later generalised to $\mathbb{Z}$-modules embedded in $\mathbb{R}^d$ [43, 96]. This provides the link for our two main topics, namely the enumeration of coincidence site lattices and similar sublattices, and its generalisation to embedded $\mathbb{Z}$-modules.

Let us give an outline of this chapter. Our main focus is on lattices and certain $\mathbb{Z}$-modules, the latter viewed as embedded in some Euclidean space. This point of view is unusual from an algebraic point of view, but motivated by the crystallographic applications to (quasi-)crystals. Therefore, all lattices are regarded as special cases of embedded $\mathbb{Z}$-modules, and one could develop the theory for embedded modules right from the beginning. However, the lattice case is without doubt such an important problem in itself that we prefer to first present the theory for lattices, and generalise later. In fact, our text is written in such a way that readers primarily interested in the lattice case can simply skip the discussions of the more general modules.

The chapter is organised as follows. We start with some basic notions and facts about lattices in Section 3.2. As a motivation and an introduction to the general theory, we consider a variety of counting problems of the square lattice in Section 3.3. This not only serves to illustrate the special enumeration problems of SSLs and CSLs we are after, but also puts them in a broader range of problems to emphasise the connections to other combinatorial questions. Section 3.4 provides some useful tools from algebra and analysis.

In Section 3.5, we discuss SSLs. After the general theory in Section 3.5.1, we consider several examples, including planar lattices (Section 3.5.2) and rational lattices in dimensions $d \geqslant 4$ (Section 3.5.3), with a detailed presentation of the lattice A_4 in Section 3.5.4 and the hypercubic lattices in Section 3.5.5. The results for lattices are finally generalised for embedded $\mathbb{Z}$-modules in Section 3.6, which also includes the icosian ring as an example (Section 3.6.1). In addition, some examples for planar modules can already be found in Section 3.5.2.

From Section 3.7 onwards, we deal with CSLs and coincidence site modules. Section 3.7 presents the general theory, both for simple and multiple CSLs. It includes a section on some connections with monotiles (Section 3.7.3). In Section 3.7.5, we generalise our results to embedded $\mathbb{Z}$-modules

and, finally, we investigate the interrelations between coincidence site modules and similar submodules in Section 3.7.6. This is followed by a series of examples. In Section 3.8, we deal with planar $\mathbb{Z}$-modules. After discussing the cubic lattices in Section 3.9, we move on to the four-dimensional hypercubic lattices in Section 3.10 and to the lattice A_4 in Section 3.11, which also covers the icosian ring as an example of a $\mathbb{Z}$-module embedded in $\mathbb{R}^4$. Section 3.12 is devoted to the multiple CSLs of the cubic lattices. Finally, we present some (rudimentary) results for dimensions $d \geqslant 5$ in Section 3.13.

Throughout this chapter, ideals play an important role. In almost all of our examples, we are dealing with principal ideals, which have a single generating element that is unique up to units. Although it is usually more elegant to formulate results in terms of ideals instead of generating elements, we will frequently prefer to deal with generating elements. The main reason is that we usually deal with ideals in algebraic number fields or quaternion algebras, and their elements can be used to parametrise rotations in dimensions $d \leqslant 4$. However, rotations are parametrised by concrete complex numbers or quaternions, respectively, and not by ideals. As we want to emphasise the direct connection to the rotations and use geometric intuition, we accept the fact that some equations are more cumbersome when formulated with quaternions and hold only up to units. For those who are more interested in an exposition using ideals, we mention [12, Sec. 5], which shows how to formulate matters in ideal-theoretic way in the context of quaternion algebras.

As we proceed, we shall prove many of the structural properties and results — in particular, when they are not trivial or not easily available in the literature. Otherwise, we state concrete results without proof, but with proper (and precise) references.

3.2. Preliminaries on lattices

Let us begin with some definitions for lattices in $\mathbb{R}^d$ (which are cocompact discrete subgroups of $\mathbb{R}^d$), where we start from the notions introduced in [AO1, Ch. 3] and refer to [23, 53] for further background. In particular, a lattice $\varGamma \subset \mathbb{R}^d$ always has full rank d (as a $\mathbb{Z}$-module), and any lattice basis can also serve as a basis for $\mathbb{R}^d$.

Definition 3.2.1. Two lattices $\varGamma_1, \varGamma_2 \subset \mathbb{R}^d$ are called *commensurate*, denoted by $\varGamma_1 \sim \varGamma_2$, if $\varGamma_1 \cap \varGamma_2$ has finite index in both $\varGamma_1$ and $\varGamma_2$.

In our terminology, commensurateness means that $\varGamma_1 \cap \varGamma_2$ is a sublattice (of full rank) of both $\varGamma_1$ and $\varGamma_2$. Actually, there are several elementary ways to characterise commensurateness [97].

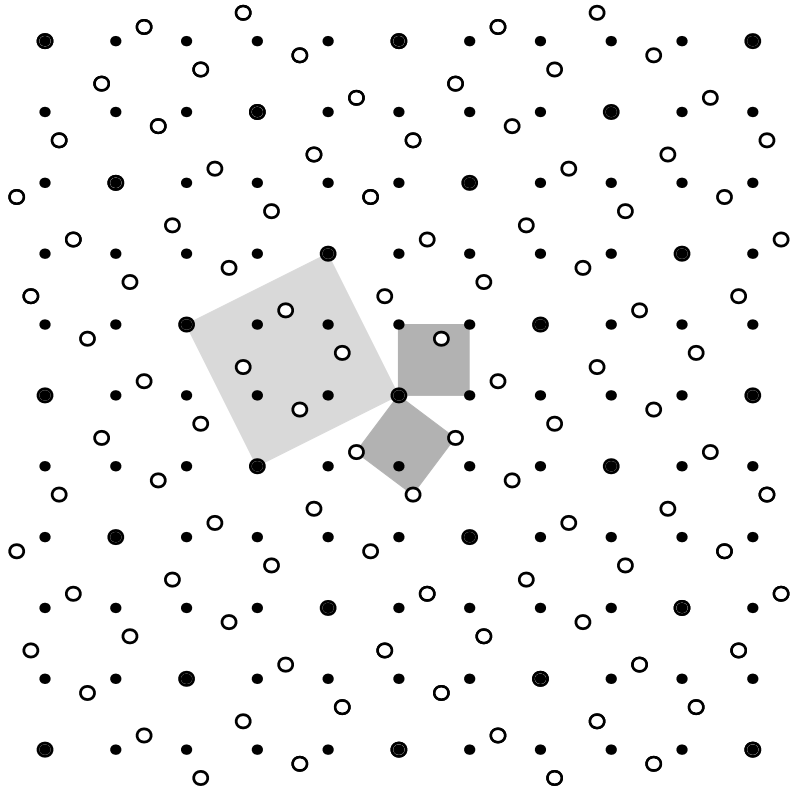

FIGURE 3.2.1. A square lattice (all black points) and a rotated copy of it (open circles together with large black points), with relative rotation angle $\alpha = \arctan(\frac{4}{3}) \approx 53.13^\circ$. The large black points mark the intersection of the two lattices, which is the CSL and again a square lattice. The shaded squares show fundamental domains of the three lattices. The larger square is a fundamental domain of the CSL.

Lemma 3.2.2. *Let Γ_1 and Γ_2 be lattices in $\mathbb{R}^d$. Then, the following statements are equivalent.*

(1) *Γ_1 and Γ_2 are commensurate.*
(2) *$\Gamma_1 \cap \Gamma_2$ has finite index in both Γ_1 and Γ_2.*
(3) *$\Gamma_1 \cap \Gamma_2$ has finite index in Γ_1 or in Γ_2.*
(4) *There exist (positive) integers m_1 and m_2 such that $m_1\Gamma_1 \subseteq \Gamma_2$ and $m_2\Gamma_2 \subseteq \Gamma_1$.*
(5) *There exists an integer $m \neq 0$ such that $m\Gamma_1 \subseteq \Gamma_2$ or $m\Gamma_2 \subseteq \Gamma_1$.*
(6) *$\Gamma_1 \cap \Gamma_2$ is a lattice (of full rank d) in $\mathbb{R}^d$.* □

As an immediate consequence, for instance via applying property (4) several times, one obtains that commensurateness is an equivalence relation.

An example of commensurate lattices is provided by similar sublattices. In fact, similarity of lattices is an important concept to us. Recall that an invertible linear map $f\colon \mathbb{R}^d \longrightarrow \mathbb{R}^d$ is called a *similarity transformation* if it is of the form $f = \alpha R$, where R is a (linear) isometry and $0 \neq \alpha \in \mathbb{R}$. Two lattices $\varGamma$ and $\varGamma'$ are called *similar*, in symbols $\varGamma \overset{\mathsf{s}}{\sim} \varGamma'$, if there exists a similarity transformation from one to the other. Clearly, similarity of lattices is an equivalence relation.

Definition 3.2.3. A similarity transformation that maps a lattice $\varGamma \in \mathbb{R}^d$ onto a sublattice of $\varGamma$ is called a *similarity transformation of* $\varGamma$. A sublattice $\varGamma' \subseteq \varGamma$ is called a *similar sublattice* (SSL) of $\varGamma$ if $\varGamma'$ is similar to $\varGamma$.

Trivial examples of SSLs are the sublattices $m\varGamma$, with $m \in \mathbb{N}$. Similarly, given an SSL $\varGamma' \subseteq \varGamma$, also $m\varGamma'$ is an SSL. In order to exclude these cases, we introduce the notion of a primitive SSL.

Definition 3.2.4. An SSL $\varGamma' \subseteq \varGamma$ is called *primitive* if $\frac{1}{n}\varGamma' \subseteq \varGamma$ with $n \in \mathbb{N}$ implies that $n = 1$.

In crystallography, the intersection $\varGamma \cap R\varGamma$ plays an important role in describing grain boundaries. If $\varGamma \cap R\varGamma$ is a lattice (of full rank), it is called a *coincidence site lattice* (CSL). A planar example is shown in Figure 3.2.1. As we have seen, the intersection $\varGamma \cap R\varGamma$ is a lattice if and only if $\varGamma$ and $R\varGamma$ are commensurate. This motivates the following definition.

Definition 3.2.5. Let $\varGamma$ be a lattice in $\mathbb{R}^d$, and let $R \in \mathrm{O}(d,\mathbb{R})$. If $\varGamma$ and $R\varGamma$ are commensurate, $\varGamma(R) := \varGamma \cap R\varGamma$ is called a *coincidence site lattice* (CSL). In this case, R is called a *coincidence isometry*. The corresponding index, $\varSigma_{\varGamma}(R) := [\varGamma : \varGamma(R)]$, is called its *coincidence index*.

Before we embark on a systematic review of CSLs and their properties, let us embed the study of such lattices, in an illustrative fashion, into a wider context that is motivated by geometry and combinatorics.

3.3. A hierarchy of planar lattice enumeration problems

It is the intention of this section to shed some more light on the coincidence problem and how it relates to various types of index-oriented sublattice enumerations with geometric constraints. Let us explain this for the square lattice in $\mathbb{R}^2$ in an informal manner. The results will be given in closed form in terms of zeta functions, and explicitly (for small indices) in Table 3.3.1 on page 81.

To this end, let us start with the question of how many sublattices of $\mathbb{Z}^2$ have index m, without any further restriction. Let us call this number a_m. Clearly, $a_1 = 1$ (only $\mathbb{Z}^2$ itself is a sublattice of index 1) and $a_2 = 3$ (counting two different rectangular sublattices and one square sublattice). In general, one has $a_{mn} = a_m a_n$ when $m, n \in \mathbb{N}$ are coprime, and one can derive, either from [4, Appendix] or from [82, Lemma 2 on p. 99], the general result that

$$a_m \,=\, \sigma_1(m) \,=\, \textstyle\sum_{d|m} d,$$

where σ_1 is a divisor function, whose Dirichlet series generating function reads

$$F(s) \,=\, \sum_{m=1}^{\infty} \frac{a_m}{m^s} \,=\, \zeta(s)\,\zeta(s-1). \tag{3.3.1}$$

Here, $\zeta(s) = \sum_{m=1}^{\infty} m^{-s}$ is Riemann's zeta function [3]. From this, it can be shown that the number of sublattices of index $\leqslant x$, which is the summatory[1] function $\sum_{k \leqslant x} a_k$, grows quadratically as $x^2\pi^2/12$; compare [54, Thm. 324]. More precisely, we have

$$\sum_{m \leqslant x} a_m \,=\, \frac{\pi^2}{12}\, x^2 + \mathcal{O}\big(x \log(x)\big) \quad \text{as } x \to \infty.$$

This counting result is, of course, *algebraic* in nature and thus applies to any planar lattice, and to the free Abelian group of rank 2 in particular (where a_m is the number of distinct subgroups of index m).

As a first geometric refinement step, let us consider those sublattices of $\mathbb{Z}^2$ which are *well-rounded*, which means that the shortest non-zero lattice vectors span the plane. Here, the result is considerably more difficult (and the most difficult one for this informal discussion), and one finds [18] that the counts $a_{\square}^{\mathsf{wr}}(m)$ lead to the Dirichlet series

$$\Phi_{\square}^{\mathsf{wr}}(s) \,=\, \Phi_{\square}^{\mathsf{pr}}(s)\big(1 + \phi_0(s) + \phi_1(s)\big), \tag{3.3.2}$$

where $\Phi_{\square}^{\mathsf{pr}}(s)$ is the generating function for all primitive square sublattices given below in Eq. (3.3.4), together with

$$\phi_0(s) \,=\, \frac{2}{2^s} \sum_{p \in \mathbb{N}} \sum_{p < q < \sqrt{3}p} \frac{1}{p^s q^s},$$

$$\phi_1(s) \,=\, \frac{2}{1+2^{-s}} \sum_{k \in \mathbb{N}} \sum_{k < \ell < \sqrt{3}k + \frac{\sqrt{3}-1}{2}} \frac{1}{(2k+1)^s (2\ell+1)^s}.$$

Although no simpler closed expressions for these functions are known, they can be approximated by explicit formulas involving Riemann's zeta function

[1] As is well known from number theory, arithmetic functions such as $m \mapsto a_m$ are prone to strong fluctuations. The corresponding summatory functions are usually more regular, and show a well-defined asymptotic behaviour; see [3] for background.

and a certain L-series [18]; see also below (Section 3.5.2) for further details. This enables us to determine the asymptotic growth rate explicitly, including an error term. As there are considerably fewer well-rounded sublattices than sublattices in total, it is not surprising that the growth rate is smaller, namely $\frac{\log(3)}{2\pi}\, x \log(x)$ as $x \to \infty$; see [18]. There exists a linear correction term, and the asymptotic behaviour reads in detail

$$\begin{aligned}\sum_{n \leqslant x} a_{\square}^{\mathsf{wr}}(n) \,&=\, \frac{\log(3)}{3}\, \frac{L(1,\chi_{-4})}{\zeta(2)}\, x\big(\log(x)-1\big) + c_{\square} x + \mathcal{O}\big(x^{3/4}\log(x)\big) \\ &=\, \frac{\log(3)}{2\pi}\, x \log(x) + \left(c_{\square} - \frac{\log(3)}{2\pi}\right) x + \mathcal{O}\big(x^{3/4}\log(x)\big),\end{aligned}$$

where, with $\gamma \approx 0.5772157$ denoting the Euler–Mascheroni constant,

$$\begin{aligned}c_{\square} \,:=\, \frac{L(1,\chi_{-4})}{\zeta(2)} \Bigg(\frac{\log(3)}{3} \left(\frac{L'(1,\chi_{-4})}{L(1,\chi_{-4})} + 3\gamma - 2\frac{\zeta'(2)}{\zeta(2)} - \frac{\log(3)}{4} - \frac{\log(2)}{6} \right) \\ + \zeta(2) - \sum_{p=1}^{\infty} \frac{1}{p} \left(\frac{\log(3)}{2} - \sum_{p<q<p\sqrt{3}} \frac{1}{q} \right) \\ - \frac{4}{3} \sum_{k=0}^{\infty} \frac{1}{2k+1} \left(\frac{1}{4}\log(3) - \sum_{k<\ell<k\sqrt{3}+\frac{\sqrt{3}-1}{2}} \frac{1}{2\ell+1} \right) \Bigg) \\ \approx\, 0.6272237.\end{aligned}$$

Note that the error term $\mathcal{O}\big(x^{3/4}\log(x)\big)$ is certainly not optimal; see [18] for more. Here, the numerical values are rounded to the last digit displayed, so that the error is less than 1 in the last digit. The same rule implicitly applies to any numerical values that we will give in the following.

Let us next ask how many of the sublattices of $\mathbb{Z}^2$ of index m are actually *square* lattices; see [7, 10, 11] for various generalisations of this question. This number can be obtained by counting the lattice points on circles of radius $\sqrt{m}$ (hence counting solutions of the Diophantine equation $x^2 + y^2 = m$) and afterwards dividing by 4 (the order of C_4, the rotation part of the point symmetry group of $\mathbb{Z}^2$). The result is given in [54, Chs. 16.9, 16.10 and 17.9] and leads to the Dirichlet series generating function

$$\Phi_{\square}(s) \,=\, \zeta_K(s) \,=\, \frac{1}{1-2^{-s}} \prod_{p \equiv 1\,(4)} \Big(\frac{1}{1-p^{-s}}\Big)^2 \prod_{p \equiv 3\,(4)} \frac{1}{1-p^{-2s}}, \tag{3.3.3}$$

where here and in what follows $\zeta_K(s) = \zeta(s)L(s,\chi_{-4})$ is the Dedekind zeta function of the quadratic field $K = \mathbb{Q}(\mathrm{i})$; compare [90, §11]. Recall that

$$L(s,\chi_{-4}) \,=\, \sum_{n=1}^{\infty} \frac{\chi_{-4}(n)}{n^s}$$

TABLE 3.3.1. Some counts of the enumeration problems for $\mathbb{Z}^2$. For indices $n \leqslant 60$, the number of multiple CSLs is the same as for CSLs, except for $n = 25$, where we have 3 multiple CSLs instead of 2 simple ones.

index m	1	2	3	4	5	6	7	8	9	10
sublattices	1	3	4	7	6	12	8	15	13	18
well-rounded	1	1	0	1	2	0	0	1	1	2
square	1	1	0	1	2	0	0	1	1	2
prim. square	1	1	0	0	2	0	0	0	0	2
coincidence	1	0	0	0	2	0	0	0	0	0
index m	11	12	13	14	15	16	17	18	19	20
sublattices	12	28	14	24	24	31	18	39	20	42
well-rounded	0	2	2	0	2	1	2	1	0	2
square	0	0	2	0	0	1	2	1	0	2
prim. square	0	0	2	0	0	0	2	0	0	0
coincidence	0	0	2	0	0	0	2	0	0	0
index m	21	22	23	24	25	26	27	28	29	30
sublattices	32	36	24	60	31	42	40	56	30	72
well-rounded	0	0	0	4	3	2	0	0	2	2
square	0	0	0	0	3	2	0	0	2	0
prim. square	0	0	0	0	2	2	0	0	2	0
coincidence	0	0	0	0	2	0	0	0	2	0
index m	31	32	33	34	35	36	37	38	39	40
sublattices	32	63	48	54	48	91	38	60	56	90
well-rounded	0	1	0	2	2	1	2	0	0	4
square	0	1	0	2	0	1	2	0	0	2
prim. square	0	0	0	2	0	0	2	0	0	0
coincidence	0	0	0	0	0	0	2	0	0	0
index m	41	42	43	44	45	46	47	48	49	50
sublattices	42	96	44	84	78	72	48	124	57	93
well-rounded	2	0	0	0	2	0	0	4	1	3
square	2	0	0	0	2	0	0	0	1	3
prim. square	2	0	0	0	0	0	0	0	0	2
coincidence	2	0	0	0	0	0	0	0	0	0
index m	51	52	53	54	55	56	57	58	59	60
sublattices	72	98	54	120	72	120	80	90	60	168
well-rounded	0	2	2	0	0	0	0	2	0	6
square	0	2	2	0	0	0	0	2	0	0
prim. square	0	0	2	0	0	0	0	2	0	0
coincidence	0	0	2	0	0	0	0	0	0	0

is the L-series for the Dirichlet character

$$\chi_{-4}(n) \,=\, \begin{cases} 0, & \text{if } n \text{ is even,} \\ 1, & \text{if } n \equiv 1 \bmod 4, \\ -1, & \text{if } n \equiv 3 \bmod 4. \end{cases}$$

The meaning of Eq. (3.3.3) becomes clear if one realises that the square sublattices of $\mathbb{Z}^2$ are precisely the non-trivial ideals of $\mathbb{Z}[\mathrm{i}]$, the ring of Gaussian integers within the quadratic field $\mathbb{Q}(\mathrm{i})$; see also [AO1, Ex. 2.15].

The growth rate of the number of similar sublattices of index $\leqslant x$ is linear, namely $\frac{\pi}{4}x$, which follows either from the asymptotic properties of $\zeta_K(s)$ near its rightmost pole (at $s = 1$) or just from counting one quarter of the lattice points inside the circle of radius $\sqrt{x}$, which is $\frac{\pi}{4}x$ to leading order in x. More precisely, one has

$$\sum_{m \leqslant x} a_{\square}(m) \,=\, \frac{\pi}{4}x + \mathcal{O}\bigl(\sqrt{x}\,\bigr);$$

see [18, Appendix] for details.

In the last case, some of the square lattices fail to be *primitive* (such as $3\mathbb{Z}^2$ etc.), which happens whenever the sublattice is an integer multiple of $\mathbb{Z}^2$ or of one of its primitive sublattices. If we exclude those, primes $p \equiv 3\ (4)$ are impossible as divisors of the index m, and some solutions of $p \equiv 1\ (4)$ also drop out (whenever the index is divisible by a square). Now, the generating function reads

$$\Phi^{\mathsf{pr}}_{\square}(s) \,=\, \bigl(1 + 2^{-s}\bigr) \prod_{p \equiv 1\ (4)} \frac{1 + p^{-s}}{1 - p^{-s}} \,=\, \frac{\zeta_K(s)}{\zeta(2s)}, \tag{3.3.4}$$

and the asymptotic growth rate of the number of primitive square sublattices of index $\leqslant x$ is again linear, this time with

$$\sum_{m \leqslant x} a^{\mathsf{pr}}_{\square}(m) \,=\, \frac{3}{2\pi}x + \mathcal{O}\bigl(\sqrt{x}\log(x)\bigr).$$

The leading term can be determined by counting one quarter of the visible points [3] in the circle of radius $\sqrt{x}$, which is $\frac{1}{4}(\pi x \frac{6}{\pi^2})$; see [18, Appendix] for the error term.

Finally, let us see how the CSLs fit into this picture. As $\mathrm{SO}(2,\mathbb{R})$ is Abelian, the symmetry group of any CSL of $\mathbb{Z}^2$ must contain a fourfold rotation, which in turn implies that the CSL must be a square lattice. Hence, any CSL is a similar sublattice. Note that this is a rather exceptional feature of the square lattice, which it shares, to our knowledge, only with the planar hexagonal lattice and some embedded modules in the plane. Nevertheless, there is a general connection between SSLs and CSLs, as we shall see in Section 3.7.6 below. Note, however, that not all square sublattices are

CSLs — they only are if they are primitive and if their index is *odd*. This finally results in the generating function of the coincidence problem described above, namely

$$\Psi_{\square}(s) \,=\, \sum_{m=1}^{\infty} \frac{a_{\square}^{\mathsf{CSL}}(m)}{m^s} \,=\, \prod_{p\equiv 1\,(4)} \frac{1+p^{-s}}{1-p^{-s}} \,=\, \bigl(1+2^{-s}\bigr)^{-1} \frac{\zeta_K(s)}{\zeta(2s)}. \tag{3.3.5}$$

As $\Psi_{\square}(s)$ differs from $\Phi_{\square}^{\mathsf{pr}}(s)$ only by the factor $(1+2^{-s})^{-1}$, the asymptotic behaviour

$$\sum_{m\leqslant x} a_{\square}^{\mathsf{CSL}}(m) \,=\, \frac{1}{\pi}\, x + \mathcal{O}\bigl(\sqrt{x}\log(x)\bigr)$$

is similar to the previous case, with the growth rate being lower by a factor of $\bigl(1+2^{-1}\bigr)^{-1} = \frac{2}{3}$. As before, this equation expresses the Dirichlet series generating function in terms of zeta functions; see Table 3.3.1 for the first few terms of the corresponding Dirichlet series. Similar formulas will also appear in many of our later examples.

Now, we may even go a step further and ask for *multiple* coincidences, i.e., intersections of any finite number of CSLs. As we shall discuss later (see Section 3.8 and, in particular, Example 3.8.5), the set of indices stays the same, but some additional lattices emerge, which are still similar sublattices, but not primitive any more.

We hope that this short digression has put the enumeration problem in a broader perspective, and also in contact with some elementary questions from analytic number theory. Of course, we are also interested in results in higher dimensions, where the picture changes significantly because $\mathrm{O}(d,\mathbb{R})$ is no longer Abelian for $d > 2$. Before we can proceed, we first need to introduce various methods and tools.

3.4. Algebraic and analytic tools

In writing the square lattice as $\mathbb{Z}^2 = \mathbb{Z}[\mathrm{i}]$, we can profit from the algebraic structure of $\mathbb{Z}[\mathrm{i}]$, which is a ring that is a *principal ideal domain* (PID). In fact, it is the ring of integers of the imaginary quadratic field $\mathbb{Q}(\mathrm{i})$, and as such the maximal order of the field. Here, the term 'order' means that we are dealing with a finitely generated $\mathbb{Z}$-module whose $\mathbb{Q}$-span is the entire field. $\mathbb{Z}[\mathrm{i}]$ is maximal for this property in the obvious sense, and unique as such.

Note that $\mathbb{Q}(\mathrm{i})$ can also be viewed as a cyclotomic field, which will later be used for an extension to analyse similar submodules and coincidence site modules of the rings $\mathbb{Z}[\xi_n]$ of integers in the cyclotomic field $\mathbb{Q}(\xi_n)$, where ξ_n is a primitive n-th root of unity. We refer to [AO1, Sec. 2.5] and to [88] for general background in this context.

As we shall see, this number-theoretic approach is truly powerful for planar structures. Consequently, one would like to have related methods also for higher-dimensional problems. This leads to a non-commutative generalisation in the form of certain quaternion algebras and their maximal orders.

3.4.1. Quaternions

As quaternions are pivotal in what follows, we briefly recall their most important properties. For details, we refer to [AO1, Sec. 2.5.4], [12, Secs. 3 and 4] and to the general literature [60, 27, 58, 54].

Let $\{\mathrm{e}, \mathrm{i}, \mathrm{j}, \mathrm{k}\}$ be the standard basis of $\mathbb{R}^4$, where

$$\mathrm{e} = (1,0,0,0), \quad \mathrm{i} = (0,1,0,0), \quad \mathrm{j} = (0,0,1,0), \quad \mathrm{k} = (0,0,0,1).$$

The *quaternion algebra* over $\mathbb{R}$ is the associative division algebra

$$\mathbb{H} := \mathbb{H}(\mathbb{R}) = \mathbb{R}\mathrm{e} + \mathbb{R}\mathrm{i} + \mathbb{R}\mathrm{j} + \mathbb{R}\mathrm{k} \simeq \mathbb{R}^4,$$

where multiplication is induced by Hamilton's relations

$$\mathrm{i}^2 = \mathrm{j}^2 = \mathrm{k}^2 = \mathrm{ijk} = -\mathrm{e}.$$

Elements of $\mathbb{H}$ are called quaternions, and a quaternion q is written as either $q = q_0\mathrm{e} + q_1\mathrm{i} + q_2\mathrm{j} + q_3\mathrm{k}$ or $q = (q_0, q_1, q_2, q_3)$. Given two quaternions q and p, their *inner product* is defined by the standard scalar product of q and p as vectors[2] in $\mathbb{R}^4$.

The *conjugate* of $q = (q_0, q_1, q_2, q_3)$ is $\overline{q} = (q_0, -q_1, -q_2, -q_3)$, and its *norm* is $\mathrm{nr}(q) = |q|^2 = q\,\overline{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2 \in \mathbb{R}$. One has $\overline{qp} = \overline{p}\,\overline{q}$ and $|q\,p|^2 = |q|^2|p|^2$ for any $q, p \in \mathbb{H}$. Given a quaternion $q = (q_0, q_1, q_2, q_3)$, its *real* and *imaginary parts* are defined as $\mathrm{Re}(q) = q_0$ and $\mathrm{Im}(q) = q_1\mathrm{i}+q_2\mathrm{j}+q_3\mathrm{k}$, respectively. It is easy to verify that $\mathrm{Re}(\mathbb{H})$ is the centre of $\mathbb{H}$, wherefore we can identify e with 1 from now on. The *imaginary space of* $\mathbb{H}$ is the three-dimensional subspace $\mathrm{Im}(\mathbb{H}) = \{\mathrm{Im}(q) \mid q \in \mathbb{H}\} \simeq \mathbb{R}^3$ of $\mathbb{H}$. For ease of notation, we will identify $\mathrm{Im}(\mathbb{H})$ and $\mathbb{R}^3$ and, in addition, also the elements $(q_1, q_2, q_3) \in \mathrm{Im}(\mathbb{H})$ with the elements $(0, q_1, q_2, q_3) \in \mathbb{H}$.

Another convenient feature of the quaternions is that they can be used to parametrise rotations in 3 and 4 dimensions; compare [60] and [12]. In $\mathbb{R}^3$, any rotation can be parametrised by a single quaternion $0 \neq q \in \mathbb{H}$ with $q = (\kappa, \lambda, \mu, \nu)$ via

$$R(q) = \frac{1}{|q|^2}\begin{pmatrix} \kappa^2+\lambda^2-\mu^2-\nu^2 & -2\kappa\nu+2\lambda\mu & 2\kappa\mu+2\lambda\nu \\ 2\kappa\nu+2\lambda\mu & \kappa^2-\lambda^2+\mu^2-\nu^2 & -2\kappa\lambda+2\mu\nu \\ -2\kappa\mu+2\lambda\nu & 2\kappa\lambda+2\mu\nu & \kappa^2-\lambda^2-\mu^2+\nu^2 \end{pmatrix}, \tag{3.4.1}$$

[2]We usually identify a quaternion $q = (q_0, q_1, q_2, q_3)$ with the corresponding row vector (q_0, q_1, q_2, q_3). However, when we use Cayley's parametrisation for rotations (see below), we will identify q with the corresponding column vector $(q_0, q_1, q_2, q_3)^T$.

where elements of $\mathbb{R}^3$ are written as column vectors. In particular, we have

$$R(q)\,x \;=\; R(q)\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \;=\; \frac{q x \bar{q}}{|q|^2}$$

for any $x \in \mathbb{R}^3$, where we have again identified x with $(0, x_1, x_2, x_3)$. Note that the parametrisation of Eq. (3.4.1), which is known as *Cayley's parametrisation*, is only unique up to a scaling factor, meaning $R(\alpha q) = R(q)$ for $\alpha \neq 0$.

As we are usually interested in specific subgroups of $\mathrm{SO}(3,\mathbb{R})$, let us mention that such subgroups often can be related to suitable subrings of $\mathbb{H}$; compare [12, Prop. 1]. In particular, the rotations of $\mathrm{SO}(3,\mathbb{Q})$ can be parametrised by integer quaternions as explained below.

In $\mathbb{R}^4$, a pair of quaternions is needed to parametrise a rotation [60, 35]. These quaternions are unique up to positive scaling factors and a common sign change. In particular,

$$R(p,q)\colon \mathbb{R}^4 \longrightarrow \mathbb{R}^4, \quad x \longmapsto R(p,q)x \;=\; \frac{p x \bar{q}}{|pq|} \tag{3.4.2}$$

defines a rotation in $\mathbb{R}^4$, whose matrix representation — in abuse of notation also written as $R(p,q) = \frac{1}{|pq|}M(p,q)$ — is explicitly given by

$$M(p,q) \;=\; \begin{pmatrix} \langle p|q\rangle & \langle p\mathrm{i}|q\rangle & \langle p\mathrm{j}|q\rangle & \langle p\mathrm{k}|q\rangle \\ \langle p|\mathrm{i}q\rangle & \langle p\mathrm{i}|\mathrm{i}q\rangle & \langle p\mathrm{j}|\mathrm{i}q\rangle & \langle p\mathrm{k}|\mathrm{i}q\rangle \\ \langle p|\mathrm{j}q\rangle & \langle p\mathrm{i}|\mathrm{j}q\rangle & \langle p\mathrm{j}|\mathrm{j}q\rangle & \langle p\mathrm{k}|\mathrm{j}q\rangle \\ \langle p|\mathrm{k}q\rangle & \langle p\mathrm{i}|\mathrm{k}q\rangle & \langle p\mathrm{j}|\mathrm{k}q\rangle & \langle p\mathrm{k}|\mathrm{k}q\rangle \end{pmatrix}$$

$$= \begin{pmatrix} ak+b\ell+cm+dn & -a\ell+bk+cn-dm & -am-bn+ck+d\ell & -an+bm-c\ell+dk \\ a\ell-bk+cn-dm & ak+b\ell-cm-dn & -an+bm+c\ell-dk & am+bn+ck+d\ell \\ am-bn-ck+d\ell & an+bm+c\ell+dk & ak-b\ell+cm-dn & -a\ell-bk+cn+dm \\ an+bm-c\ell-dk & -am+bn-ck+d\ell & a\ell+bk+cn+dm & ak-b\ell-cm+dn \end{pmatrix},$$

where $p = (k,\ell,m,n)$ and $q = (a,b,c,d)$. Here, $\langle\cdot|\cdot\rangle$ denotes the standard inner product in $\mathbb{R}^4$.

A quaternion all of whose components are integers is called a *Lipschitz quaternion*. The set $\mathbb{L}$ of Lipschitz quaternions is thus defined as

$$\mathbb{L} \;:=\; \big\{(q_0,q_1,q_2,q_3) \in \mathbb{H} \;\big|\; q_0,q_1,q_2,q_3 \in \mathbb{Z}\big\}. \tag{3.4.3}$$

The Lipschitz quaternions form an order in the quaternion algebra $\mathbb{H}(\mathbb{Q})$, but not a maximal one. A *primitive Lipschitz quaternion* q is a quaternion in $\mathbb{L}$ whose components are relatively prime. Furthermore, a *Hurwitz quaternion* is a quaternion whose components are all integers or all half-integers. The ring $\mathbb{J}$ of Hurwitz quaternions [58] is a maximal order in the quaternion algebra $\mathbb{H}(\mathbb{Q})$, as is any of its conjugates (which means that one only has uniqueness

up to conjugacy here). $\mathbb{J}$ is given by

$$\begin{aligned}\mathbb{J} &:= \left\{(q_0,q_1,q_2,q_3) \in \mathbb{H} \;\middle|\; \text{all } q_i \in \mathbb{Z} \text{ or all } q_i \in \tfrac{1}{2}+\mathbb{Z}\right\} \\ &= \mathbb{L} \cup \left((\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+\mathbb{L}\right);\end{aligned} \tag{3.4.4}$$

compare [AO1, Ex. 2.18]. We call a Hurwitz quaternion $q \in \mathbb{J}$ *primitive* if $\frac{1}{n}q \in \mathbb{J}$ with $n \in \mathbb{N}$ implies $n = 1$. The norm $|q|^2$ of any Hurwitz quaternion is an integer. As quaternions of norm $|q|^2 = 2$ play a special role in $\mathbb{J}$, we distinguish between *odd* and *even* quaternions, where $q \in \mathbb{J}$ is called even or odd depending on whether $|q|^2$ is even or odd. Any quaternion of norm $|q|^2 = 2$ can be represented as $q = (1,1,0,0)u = u'(1,1,0,0)$, where u, u' are unit quaternions. As the group $\mathbb{J}^\times$ of unit quaternions has order 24 and consists of the quaternions

$$(\pm 1,0,0,0),(0,\pm 1,0,0),(0,0,\pm 1,0),(0,0,0,\pm 1) \text{ and } (\pm 1,\pm 1,\pm 1,\pm 1),$$

there are also 24 quaternions of norm $|q|^2 = 2$. The latter, normalised as $\frac{q}{\sqrt{2}}$, together with the units $u \in \mathbb{J}^\times$ form a group of order 48, which is a double cover of the octahedral group O.

Recall from [58] and [AO1, Sec. 2.5.4] that $\mathbb{J}$ is a principal ideal ring, which here means that all right (left) ideals are principal right (left) ideals, and $\mathbb{J}$ is also a maximal order. Thus, for any two right ideals $a\mathbb{J}$ and $b\mathbb{J}$, there exist quaternions g and m such that $g\mathbb{J} = a\mathbb{J} + b\mathbb{J}$ and $m\mathbb{J} = a\mathbb{J} \cap b\mathbb{J}$. These two quaternions g and m are unique up to multiplication by a unit quaternion from the right. We call g a *greatest common left divisor* of a and b, and m a *least common right multiple* of a and b, in symbols $g = \mathrm{gcld}(a,b)$ and $m = \mathrm{lcrm}(a,b)$. As g and m are unique only up to a unit, these equations only make sense as a shorthand notation for the corresponding equation of ideals $g\mathbb{J} = \mathrm{gcld}(a,b)\mathbb{J}$ or as equations of quaternions that hold up to a multiplication by a unit quaternion from the right. In some cases, we may choose a particular g or m. In these cases, the equations involving them are considered to hold exactly. Similarly, we define the *greatest common right divisor* gcrd and the *least common left multiple* lclm.

Similarly, the icosian ring $\mathbb{I}$ is a maximal order in $\mathbb{H}(\mathbb{Q}(\sqrt{5}))$; we refer to [AO1, Ex. 2.19] for the definition. The above notions can thus analogously be defined for $\mathbb{I}$. One important difference will emerge from the existence of another maximal order, $\mathbb{I}'$, which is obtained from $\mathbb{I}$ by algebraic conjugation in $\mathbb{Q}(\sqrt{5})$, though it is not of the form $q\mathbb{I}q^{-1}$. Here, the group of units $\mathbb{I}^\times$ is infinite and isomorphic to $\mathbb{Z}[\tau]^\times \times \Delta_{H_4}$, where Δ_{H_4} is a group of order 120; see [AO1, Ex. 2.19] for details.

For further properties of maximal orders in quaternion algebras, we refer to [76, 86]; see also [12, Sec. 4], where the case of $\mathbb{H}(K)$ with K a real algebraic number field is considered in more detail.

3.4.2. Tools from analysis

In our enumeration problems, we naturally deal with arithmetic functions $a(m)$, which are functions defined on $\mathbb{N}$. In many examples, these functions are *multiplicative*, which means that $a(mn) = a(m)\,a(n)$ whenever m and n are coprime. Note that, unless $a \equiv 0$, this implies $a(1) = 1$, and a is then completely determined by its values for p^n with p prime and $n \geqslant 1$.

In addition, we are often interested in the *summatory function*

$$A(x) \,=\, \sum_{m \leqslant x} a(m)$$

and its behaviour for large x, as this function behaves more regularly than $a(m)$ itself. This suggests to use generating functions and to analyse their analytic properties. In the context of multiplicative functions (although not restricted to those), a natural choice for the generating function is a *Dirichlet series* of the form $F(s) = \sum_{m=1}^{\infty} a(m) m^{-s}$. Let us recall one classic result for the case that $a(m)$ is real and non-negative, which relates $F(s)$ with the asymptotic behaviour of $A(x)$.

Theorem 3.4.1. *Let $F(s)$ be a Dirichlet series with non-negative coefficients which converges for $\mathrm{Re}(s) > \alpha > 0$. Suppose that $F(s)$ is holomorphic at all points of the line $\{\mathrm{Re}(s) = \alpha\}$ except at $s = \alpha$. Here, when approaching α from the half-plane to the right of it, we assume $F(s)$ to have a singularity of the form $F(s) = h(s)/(s-\alpha)^{n+1}$ where n is a non-negative integer, and $h(s)$ is holomorphic at $s = \alpha$. Then, as $x \to \infty$, we have*

$$A(x) \,:=\, \sum_{m \leqslant x} a(m) \;\sim\; \frac{h(\alpha)}{\alpha \cdot n!}\, x^{\alpha} \big(\log(x)\big)^{n}. \qquad \square$$

The proof follows easily from Delange's theorem, for instance by taking $q = 0$ and $\omega = n$ in Tenenbaum's formulation; see [85, Ch. II.7, Thm. 15] and references given there.

3.5. Similar sublattices

3.5.1. General results

Let us now have a more detailed look at similar sublattices. A similarity transformation consists of two ingredients, an isometry and a scaling factor. It thus makes sense to analyse these two parts independently and to introduce the following notions. We call

$$\mathrm{OS}(\varGamma) \,:=\, \{R \in \mathrm{O}(d,\mathbb{R}) \mid \exists \alpha \in \mathbb{R}_+ \text{ such that } \alpha R \varGamma \subseteq \varGamma\} \tag{3.5.1}$$

the set of all *similarity isometries* of $\varGamma$. Likewise, we define

$$\mathrm{SOS}(\varGamma) \,:=\, \mathrm{OS}(\varGamma) \cap \mathrm{SO}(d,\mathbb{R}) \tag{3.5.2}$$

to be its orientation-preserving part. The following result is immediate.

Fact 3.5.1. *$\mathrm{OS}(\Gamma)$ and $\mathrm{SOS}(\Gamma)$ are subgroups of $\mathrm{O}(d,\mathbb{R})$.* □

One would expect that similar lattices should have related OS-groups, which is indeed true.

Lemma 3.5.2. *Let Γ and Γ' be similar lattices with $\Gamma' = \alpha R\Gamma$. Then,*

$$\mathrm{OS}(\Gamma') \;=\; R\,\mathrm{OS}(\Gamma)\,R^{-1}.$$

Proof. If $\alpha \neq 0$, the relation $\mathrm{OS}(\Gamma) = \mathrm{OS}(\alpha\Gamma)$ is trivial. The general case follows from the fact that $\beta S\Gamma \subseteq \Gamma$ holds if and only if $\beta RSR^{-1}\Gamma' \subseteq \Gamma'$. □

Next, we aim to gain some insight into the scaling factors. Let us define

$$\begin{aligned} \mathrm{Scal}_{\Gamma}(R) &:= \{\alpha \in \mathbb{R} \mid \alpha R\Gamma \subseteq \Gamma\} \quad \text{and} \\ \mathrm{scal}_{\Gamma}(R) &:= \{\alpha \in \mathbb{R} \mid \alpha R\Gamma \sim \Gamma\}. \end{aligned} \tag{3.5.3}$$

Note that we have allowed negative values for the scaling factors here. For an arbitrary but fixed $R \in \mathrm{O}(d,\mathbb{R})$, this ensures that $\mathrm{Scal}_{\Gamma}(R)$ is a $\mathbb{Z}$-module and that $\mathrm{scal}_{\Gamma}(R) \cup \{0\}$ is a vector space over the field $\mathbb{Q}$. As we shall see shortly, this vector space is one-dimensional if $R \in \mathrm{OS}(\Gamma)$, and $\mathrm{Scal}_{\Gamma}(R)$ is then a one-dimensional lattice.

We defined $\mathrm{Scal}_{\Gamma}(R)$ and $\mathrm{scal}_{\Gamma}(R)$ for arbitrary $R \in \mathrm{O}(d,\mathbb{R})$. However, we are really only interested in the non-trivial case where $R \in \mathrm{OS}(\Gamma)$. Clearly, the scaling factor 0 is always contained in $\mathrm{Scal}_{\Gamma}(R)$, so $\mathrm{Scal}_{\Gamma}(R)$ is always non-empty. By definition, $R \in \mathrm{OS}(\Gamma)$ if and only if there exists an $\alpha \in \mathbb{R}_+$ such that $\alpha R\Gamma \subseteq \Gamma$. Hence, we have the following elementary result.

Fact 3.5.3 ([42, Sec. 4])**.** *Let Γ be a lattice in $\mathbb{R}^d$ and $R \in \mathrm{O}(d,\mathbb{R})$. Then, the following assertions are equivalent.*

(1) $\mathrm{Scal}_{\Gamma}(R) \neq \{0\}$;
(2) $\mathrm{scal}_{\Gamma}(R) \neq \varnothing$;
(3) $R \in \mathrm{OS}(\Gamma)$. □

One expects that two similar lattices should display the same sets of scaling factors. Indeed, one has the following result.

Lemma 3.5.4. *Let Γ and Γ' be similar lattices, with $\Gamma' = \alpha R\Gamma$. Then,*

$$\mathrm{Scal}_{\Gamma'}(S) \;=\; \mathrm{Scal}_{\Gamma}(R^{-1}SR) \quad \textit{and} \quad \mathrm{scal}_{\Gamma'}(S) \;=\; \mathrm{scal}_{\Gamma}(R^{-1}SR).$$

Proof. Let $\beta \in \mathrm{Scal}_{\Gamma'}(S)$, so that $\beta S\Gamma' \subseteq \Gamma' = \alpha R\Gamma$. This is equivalent to $\beta R^{-1}SR\Gamma \subseteq \Gamma$, from which we infer the first identity. The second one follows similarly. □

For a fixed lattice $\Gamma \subset \mathbb{R}^d$, let us have a closer look at the elements of $\mathrm{Scal}_\Gamma(R)$. By basic facts from linear algebra, we have

$$[\Gamma : \alpha R\Gamma] = |\det(\alpha R)| = \alpha^d |\det(R)| = \alpha^d,$$

whenever αR is a similarity transformation of Γ. Hence, α^d must be an integer for all $\alpha \in \mathrm{Scal}_\Gamma(R)$. More generally, if $\alpha R\Gamma \sim \Gamma$, there exists an integer m such that $m\alpha R\Gamma$ is a similar sublattice of Γ. Consequently, we have $\alpha^d \in \mathbb{Q}$ whenever $\alpha \in \mathrm{scal}_\Gamma(R)$. We have thus proved the following.

Lemma 3.5.5. *Let $\Gamma \subset \mathbb{R}^d$ be a lattice. For any $\alpha \in \mathrm{Scal}_\Gamma(R)$, we have $\alpha^d \in \mathbb{Z}$. Moreover, for any $\alpha \in \mathrm{scal}_\Gamma(R)$, we have $\alpha^d \in \mathbb{Q}$.* □

As a consequence, for any fixed lattice Γ, $\mathrm{Scal}_\Gamma(R)$ is a discrete and closed set, or in other words, a locally finite set. Hence, there exists a smallest positive element in $\mathrm{Scal}_\Gamma(R)$. This deserves a name.

Definition 3.5.6. For any isometry $R \in \mathrm{OS}(\Gamma)$, the smallest positive element in $\mathrm{Scal}_\Gamma(R)$ is called the *denominator* of R, written as $\mathrm{den}_\Gamma(R)$.

Clearly, one has $\big(\mathrm{den}_\Gamma(R)\big)^d \in \mathbb{N}$. Moreover, $\mathrm{den}_\Gamma(R) = 1$ is equivalent to $R\Gamma = \Gamma$, that is, $\mathrm{den}_\Gamma(R) = 1$ if and only if R is a symmetry operation of the lattice Γ. In particular, $\mathrm{den}_\Gamma(\mathbb{1}) = 1$.

As $\mathrm{Scal}_\Gamma(R)$ is a $\mathbb{Z}$-module, each integer multiple of $\mathrm{den}_\Gamma(R)$ is again an element of $\mathrm{Scal}_\Gamma(R)$. On the other hand, each $\alpha \in \mathrm{Scal}_\Gamma(R)$ must be a multiple of $\mathrm{den}_\Gamma(R)$, since otherwise we could find a scaling factor α with $0 < \alpha < \mathrm{den}_\Gamma(R)$. This leads to the following result.

Lemma 3.5.7. *Let $\Gamma \subset \mathbb{R}^d$ be a lattice. For any isometry $R \in \mathrm{OS}(\Gamma)$, we have $\mathrm{Scal}_\Gamma(R) = \mathrm{den}_\Gamma(R)\,\mathbb{Z}$ and $\mathrm{scal}_\Gamma(R) = \mathrm{den}_\Gamma(R)\,\mathbb{Q}^\times$.*

Proof. It remains to prove the statement about $\mathrm{scal}_\Gamma(R)$. By definition, $\alpha \in \mathrm{scal}_\Gamma(R)$ means $\alpha R\Gamma \sim \Gamma$. By Lemma 3.2.2, there exists an $m \in \mathbb{N}$ such that $m\alpha R\Gamma \subseteq \Gamma$, whence $m\alpha \in \mathrm{Scal}_\Gamma(R) = \mathrm{den}_\Gamma(R)\,\mathbb{Z}$ and thus also $\mathrm{scal}_\Gamma(R) \subseteq \mathrm{den}_\Gamma(R)\,\mathbb{Q}^\times$. On the other hand, $\mathrm{den}_\Gamma(R)R\Gamma \sim \Gamma$ and $q\Gamma \sim \Gamma$ for all $q \in \mathbb{Q}$ imply that $\alpha R\Gamma \sim \Gamma$ for all $\alpha \in \mathrm{den}_\Gamma(R)\,\mathbb{Q}^\times$, which shows that $\mathrm{scal}_\Gamma(R) \supseteq \mathrm{den}_\Gamma(R)\,\mathbb{Q}^\times$ as well. □

More generally, we have $\mathrm{scal}_\Gamma(R) = \alpha\mathbb{Q}^\times$ for any $\alpha \in \mathrm{scal}_\Gamma(R)$. Note that $\mathrm{scal}_\Gamma(\mathbb{1}) = \mathbb{Q}^\times$ and $\mathrm{Scal}_\Gamma(\mathbb{1}) = \mathbb{Z}$.

Although we are ultimately more interested in the sets $\mathrm{Scal}_\Gamma(R)$, it is worthwhile to discuss $\mathrm{scal}_\Gamma(R)$ as these sets are easier to handle. In particular, we have a natural group structure on $\{\mathrm{scal}_\Gamma(R) \mid R \in \mathrm{OS}(\Gamma)\}$, with the product of two sets A and B defined as $AB := \{\alpha\beta \mid \alpha \in A, \beta \in B\}$, and the inverse of A given by $A^{-1} = \{\alpha^{-1} \mid \alpha \in A\}$. The latter is well defined as $0 \notin A$ whenever $A = \mathrm{scal}_\Gamma(R)$.

Lemma 3.5.8. *Let $\varGamma \subset \mathbb{R}^d$ be a lattice. For any $R, S \in \mathrm{OS}(\varGamma)$, we have*

$$\mathrm{scal}_{\varGamma}(R)\,\mathrm{scal}_{\varGamma}(S) \,=\, \mathrm{scal}_{\varGamma}(RS) \quad \textit{and} \quad \mathrm{scal}_{\varGamma}(R^{-1}) \,=\, \bigl(\mathrm{scal}_{\varGamma}(R)\bigr)^{-1}.$$

Proof. The group structure is a consequence of the fact that commensurateness is an equivalence relation. Alternatively, this property also follows from Lemma 3.5.7, which suggests the definition of a natural mapping from the set $\{\mathrm{scal}_{\varGamma}(R) \mid R \in \mathrm{OS}(\varGamma)\}$ into the multiplicative group $\mathbb{R}_+/\mathbb{Q}_+$, which becomes a group homomorphism with the multiplication as defined in this lemma. □

Actually, it is the homomorphism mentioned in the previous proof that will establish a general connection between SSLs and CSLs, as we shall discuss in Section 3.7.6.

Note that $\{\mathrm{scal}_{\varGamma}(R) \mid R \in \mathrm{OS}(\varGamma)\}$ is an Abelian group, although $\mathrm{OS}(\varGamma)$ is not Abelian in general. In particular, one has $\mathrm{scal}_{\varGamma}(RS) = \mathrm{scal}_{\varGamma}(SR)$ even when $RS \neq SR$.

The situation is more involved for the sets $\mathrm{Scal}_{\varGamma}(R)$. They do not form a group, nor even a semigroup, as $\mathrm{Scal}_{\varGamma}(R)\,\mathrm{Scal}_{\varGamma}(S) \subseteq \mathrm{Scal}_{\varGamma}(RS)$ is usually a proper inclusion. Nevertheless, we can still extract some information on the denominator from this inclusion; compare [96, 97]. As $\mathrm{den}_{\varGamma}(R)\,\mathrm{den}_{\varGamma}(S)$ must be in $\mathrm{scal}_{\varGamma}(RS)$, it is an integer multiple of $\mathrm{den}_{\varGamma}(RS)$, that is,

$$\frac{\mathrm{den}_{\varGamma}(R)\,\mathrm{den}_{\varGamma}(S)}{\mathrm{den}_{\varGamma}(RS)} \,\in\, \mathbb{N}. \tag{3.5.4}$$

An immediate consequence is that $\mathrm{den}_{\varGamma}(R)\,\mathrm{den}_{\varGamma}(R^{-1})$ is an integer. Moreover, as $[\varGamma : \mathrm{den}_{\varGamma}(R)R\varGamma] = \bigl(\mathrm{den}_{\varGamma}(R)\bigr)^d$ for an isometry $R \in \mathrm{OS}(\varGamma)$, we have $\bigl(\mathrm{den}_{\varGamma}(R)\bigr)^d \varGamma \subseteq \mathrm{den}_{\varGamma}(R)R\varGamma$, from which we infer $\bigl(\mathrm{den}_{\varGamma}(R)\bigr)^{d-1} R^{-1}\varGamma \subseteq \varGamma$. This proves

$$\frac{\bigl(\mathrm{den}_{\varGamma}(R)\bigr)^{d-1}}{\mathrm{den}_{\varGamma}(R^{-1})} \,\in\, \mathbb{N}. \tag{3.5.5}$$

Remark 3.5.9. Formula (3.5.5) implies $\mathrm{den}_{\varGamma}(R^{-1}) \leqslant \bigl(\mathrm{den}_{\varGamma}(R)\bigr)^{d-1}$. In fact, this upper bound is sharp. As an example, we consider the $\mathbb{Z}$-span of the vectors $\xi^{i-1}e_i$, where ξ is the (positive) d-th root of a positive integer and $\{e_1, \ldots, e_d\}$ is an orthonormal basis of $\mathbb{R}^d$. Let R be the rotation that maps e_i onto e_{i+1} for $1 \leqslant i \leqslant d-1$ and e_d onto e_1. Then, $\mathrm{den}_{\varGamma}(R) = \xi$ and $\mathrm{den}_{\varGamma}(R^{-1}) = \xi^{d-1}$. ◊

The example in Remark 3.5.9 also shows that $\mathrm{den}_{\varGamma}(R)$ and $\mathrm{den}_{\varGamma}(R^{-1})$ generally differ if $d \geqslant 3$. However, in two dimensions, they always agree.

Corollary 3.5.10. *For any planar lattice $\varGamma$, one has* $\mathrm{den}_{\varGamma}(R^{-1}) = \mathrm{den}_{\varGamma}(R)$.

PROOF. From Eq. (3.5.5), we infer

$$\frac{\operatorname{den}_\Gamma(R)}{\operatorname{den}_\Gamma(R^{-1})} \in \mathbb{N} \quad \text{as well as} \quad \frac{\operatorname{den}_\Gamma(R^{-1})}{\operatorname{den}_\Gamma(R)} \in \mathbb{N},$$

the latter by symmetry. Together, they imply $\operatorname{den}_\Gamma(R^{-1}) = \operatorname{den}_\Gamma(R)$. □

It is quite useful to understand the relationship between commensurate lattices in more detail. Using the fact that commensurateness is an equivalence relation, we can prove the following result.

Lemma 3.5.11. *If Γ and Γ' are two commensurate lattices in $\mathbb{R}^d$, one has $\operatorname{OS}(\Gamma) = \operatorname{OS}(\Gamma')$ as well as $\operatorname{scal}_\Gamma(R) = \operatorname{scal}_{\Gamma'}(R)$.*

PROOF. By Fact 3.5.3, $R \in \operatorname{OS}(\Gamma)$ if and only if there exists an $\alpha \neq 0$ such that $\alpha R\Gamma \subseteq \Gamma$. Commensurateness guarantees that there are $m, n \in \mathbb{N}$ such that $m\Gamma \subseteq \Gamma'$ and $n\Gamma' \subseteq \Gamma$. Thus, $\alpha R\Gamma \subseteq \Gamma$ implies

$$mn\alpha R\Gamma' \subseteq m\alpha R\Gamma \subseteq m\Gamma \subseteq \Gamma', \tag{3.5.6}$$

which gives $\operatorname{OS}(\Gamma) \subseteq \operatorname{OS}(\Gamma')$. By symmetry, we conclude $\operatorname{OS}(\Gamma) = \operatorname{OS}(\Gamma')$. Moreover, Eq. (3.5.6) shows that $\operatorname{den}_\Gamma(R)$ and $\operatorname{den}_{\Gamma'}(R)$ differ only by a factor $q \in \mathbb{Q}$, whence $\operatorname{scal}_\Gamma(R) = \operatorname{scal}_{\Gamma'}(R)$ by Lemma 3.5.7. □

Of course, we cannot expect the sets $\operatorname{Scal}_\Gamma(R)$ and $\operatorname{Scal}_{\Gamma'}(R)$ to be equal. However, as we can sandwich Γ' between appropriately scaled copies of Γ, we can derive lower and upper bounds as follows.

Proposition 3.5.12. *Let Γ' be a sublattice of Γ of index m. Then,*

$$m \operatorname{Scal}_\Gamma(R) \subseteq \operatorname{Scal}_{\Gamma'}(R) \subseteq \frac{1}{m} \operatorname{Scal}_\Gamma(R).$$

Moreover, one has

$$\frac{m \operatorname{den}_\Gamma(R)}{\operatorname{den}_{\Gamma'}(R)} \in \mathbb{N} \quad \text{and} \quad \frac{m \operatorname{den}_{\Gamma'}(R)}{\operatorname{den}_\Gamma(R)} \in \mathbb{N}.$$

PROOF. If $\alpha \in \operatorname{Scal}_\Gamma(R)$, then

$$\alpha R\Gamma' \subseteq \alpha R\Gamma \subseteq \Gamma \subseteq \tfrac{1}{m}\Gamma'$$

shows that $m\alpha \in \operatorname{Scal}_{\Gamma'}(R)$. Similarly, $\alpha \in \operatorname{Scal}_{\Gamma'}(R)$ implies

$$\alpha Rm\Gamma \subseteq \alpha R\Gamma' \subseteq \Gamma' \subseteq \Gamma,$$

which proves $\operatorname{Scal}_{\Gamma'}(R) \subseteq \frac{1}{m} \operatorname{Scal}_\Gamma(R)$. The statement about the denominators now follows from the explicit expressions for $\operatorname{Scal}_\Gamma(R)$ from Lemma 3.5.7, or by choosing α to be the denominator in the equations above. □

Let us add that, more generally, one can show that

$$m_1 m_2 \operatorname{Scal}_\Gamma(R) \subseteq \operatorname{Scal}_{\Gamma'}(R) \subseteq \frac{1}{m_1 m_2} \operatorname{Scal}_\Gamma(R)$$

whenever $m_1\varGamma \subseteq \varGamma'$ and $m_2\varGamma' \subseteq \varGamma$.

Let us conclude these general considerations with a remark on the dual lattice, $\varGamma^* = \{x \in \mathbb{R}^d \mid \langle x|y\rangle \in \mathbb{Z} \text{ for all } y \in \varGamma\}$; compare [AO1, Sec. 3.1].

Lemma 3.5.13. *If $\varGamma^*$ is the dual lattice of $\varGamma$, one has* $\mathrm{OS}(\varGamma) = \mathrm{OS}(\varGamma^*)$ *together with*

$$\mathrm{Scal}_{\varGamma^*}(R) \,=\, \mathrm{Scal}_{\varGamma}(R^{-1}).$$

In particular, $\mathrm{den}_{\varGamma^*}(R) = \mathrm{den}_{\varGamma}(R^{-1})$.

Proof. As $\mathrm{OS}(\varGamma)$ is a group, $R \in \mathrm{OS}(\varGamma)$ if and only if $R^{-1} \in \mathrm{OS}(\varGamma)$. The latter holds if and only if there is an $\alpha \in \mathbb{R}_+$ such that $\alpha R^{-1}\varGamma \subseteq \varGamma$. By the definition of the dual lattice, this is equivalent to $\alpha\langle x|R^{-1}y\rangle \in \mathbb{Z}$ for all $x \in \varGamma^*$ and $y \in \varGamma$.

Now, $\alpha\langle Rx|y\rangle = \alpha\langle x|R^{-1}y\rangle$ shows that $\alpha R\varGamma^* \subseteq \varGamma^*$ holds if and only if $\alpha R^{-1}\varGamma \subseteq \varGamma$, which proves $\mathrm{OS}(\varGamma) = \mathrm{OS}(\varGamma^*)$. On the other hand, this equation shows that $\alpha \in \mathrm{Scal}_{\varGamma^*}(R)$ if and only if $\alpha \in \mathrm{Scal}_{\varGamma}(R^{-1})$, which completes the proof. □

3.5.2. Two dimensions

Let us consider some concrete examples. We start in two dimensions, where we can make use of the field of complex numbers to characterise $\mathrm{SOS}(\varGamma)$ completely. Here, any orientation-preserving similarity transformation can be represented by complex multiplication, and it turns out that the semigroup of similarity transformations then forms a ring, which we call the *multiplier ring*. The latter is denoted by $\mathrm{MR}(\varGamma)$. Actually, there are only two cases. Either $\mathrm{SOS}(\varGamma) = \{\pm 1\}$, or equivalently $\mathrm{MR}(\varGamma) = \mathbb{Z}$, in which case we call $\varGamma$ *generic*, or $\mathrm{MR}(\varGamma) = \mathcal{O}$ is an order[3] in an imaginary quadratic number field; compare [17] and [54, 21, 29] for general background.

For a more precise formulation, we employ the *similarity class* of a given lattice $\varGamma$, denoted by $\mathrm{sim}(\varGamma)$, which consists of all lattices $\varGamma' \sim \varGamma$.

Theorem 3.5.14 ([17, Prop. 2.3 and Thm. 2.6])**.** *If $\varGamma \subset \mathbb{R}^2$ is a non-generic lattice, its multiplier ring* $\mathrm{MR}(\varGamma)$ *is an order in an imaginary quadratic field. Explicitly, if $\varGamma \in \mathrm{sim}\big(\langle 1, \tau\rangle_{\mathbb{Z}}\big)$ with $\tau \in \mathbb{C} \setminus \mathbb{R}$ is a non-generic lattice, the number τ is algebraic of degree 2 over $\mathbb{Q}$, and one has*

$$\mathrm{MR}(\varGamma) \,=\, \langle 1, s\tau\rangle_{\mathbb{Z}}$$

for some non-zero integer s.

[3]Note that the symbol $\mathcal{O}$ occurs with two different meanings in this chapter, namely for asymptotic estimates and for orders (in the algebraic sense introduced earlier). Since the meaning will always be clear from the context, we stick to this widely used notation.

Moreover, if K is the field of fractions of $\mathcal{O} := \mathrm{MR}(\Gamma)$, we have the relation $\mathrm{MR}(\Gamma) = \mathcal{O} = \mathrm{MR}(\mathcal{O})$. In particular,

$$\begin{aligned}\mathrm{SOS}(\Gamma) \;&=\; \mathrm{SOS}(\mathcal{O}) \;=\; \mathrm{SOS}(\mathcal{O}_K)\\ &=\; \Big\{ \frac{w}{|w|} \;\Big|\; 0 \neq w \in \mathcal{O} \Big\} \;=\; \Big\{ \frac{w}{|w|} \;\Big|\; 0 \neq w \in \mathcal{O}_K \Big\},\end{aligned}$$

where $\mathcal{O}_K$ is the maximal order of K and thus contains $\mathcal{O}$. □

Note that the group $\mathrm{SOS}(\Gamma)$ is the same for all lattices in $\mathrm{sim}(\Gamma)$, which follows via Lemma 3.5.2 from the fact that the group $\mathrm{SO}(2)$ is Abelian. Actually, it is the same for all lattices whose multiplier ring has the same field of fractions, although the corresponding multiplier rings usually differ.

Example 3.5.15. For the square lattice, which we write as $\mathbb{Z}^2 = \mathbb{Z}[\mathrm{i}]$, we have $\mathrm{MR}\big(\mathbb{Z}[\mathrm{i}]\big) = \mathbb{Z}[\mathrm{i}]$. This implies

$$\mathrm{SOS}\big(\mathbb{Z}[\mathrm{i}]\big) \;=\; \Big\{ \frac{z}{|z|} \;\Big|\; 0 \neq z \in \mathbb{Z}[\mathrm{i}] \Big\} \;\simeq\; C_8 \times \mathbb{Z}^{(\aleph_0)},$$

where $\mathbb{Z}^{(\aleph_0)}$ denotes the countably infinite sum of infinite cyclic groups (in contrast to the infinite product). Here, the group C_8 is generated by $\frac{1+\mathrm{i}}{\sqrt{2}}$ and contains all units of $\mathbb{Z}[\mathrm{i}]$, whereas a full set of generators of $\mathbb{Z}^{(\aleph_0)}$ is the set $\big\{ \frac{\pi_p}{\sqrt{p}} \mid p \equiv 1 \bmod 4 \big\}$, where π_p is a Gaussian prime such that $\pi_p \overline{\pi_p} = p$. Note that for any p only one prime of the pair π_p, $\overline{\pi_p}$ is needed, as we have $\big(\frac{\pi_p}{\sqrt{p}}\big)^{-1} = \frac{\overline{\pi_p}}{\sqrt{p}}$. ◊

The situation is particularly nice if the multiplier ring is a PID. In this case, all ideals are similar sublattices and the situation is completely analogous to that of the square lattice example in Section 3.3, so we can write down the generating function explicitly. This happens for a finite number of cases only; compare Table 3.5.1.

Lemma 3.5.16 ([29, Thm. 7.30])**.** *There are precisely nine imaginary quadratic fields with class number 1, which means that their maximal orders are PIDs. These are the fields $K = \mathbb{Q}(\omega_0)$ for*

$$\omega_0 \;\in\; \big\{ \tfrac{1+\mathrm{i}\sqrt{3}}{2}, \mathrm{i}, \tfrac{1+\mathrm{i}\sqrt{7}}{2}, \mathrm{i}\sqrt{2}, \tfrac{1+\mathrm{i}\sqrt{11}}{2}, \tfrac{1+\mathrm{i}\sqrt{19}}{2}, \tfrac{1+\mathrm{i}\sqrt{43}}{2}, \tfrac{1+\mathrm{i}\sqrt{67}}{2}, \tfrac{1+\mathrm{i}\sqrt{163}}{2} \big\},$$

which are fields of discriminant

$$d_K \in \{-3, -4, -7, -8, -11, -19, -43, -67, -163\}.$$

In this formulation, the maximal order of K is $\mathcal{O}_K = \mathbb{Z}[\omega_0]$, while one has $\mathbb{Q}(\omega_0) = \mathbb{Q}(\sqrt{d_K}\,)$. □

Remark 3.5.17. In the nine cases of Lemma 3.5.16, the possible indices of the similar sublattices of $\mathcal{O}_K$ are precisely those positive integers that can

TABLE 3.5.1. Norm forms for the nine maximal orders $\mathcal{O}_K$ of class number 1 in imaginary quadratic number fields, labelled with the field discriminant d_K; see Lemma 3.5.16 and Remark 3.5.17 for details.

d_K	norm form	d_K	norm form	d_K	norm form
-3	x^2+xy+y^2	-8	x^2+2y^2	-43	$x^2+xy+11y^2$
-4	x^2+y^2	-11	$x^2+xy+3y^2$	-67	$x^2+xy+17y^2$
-7	$x^2+xy+2y^2$	-19	$x^2+xy+5y^2$	-163	$x^2+xy+41y^2$

be represented by the corresponding norm forms listed in Table 3.5.1. As a consequence, the Dirichlet series generating function for the number of SSLs of a given index is the zeta function of $\mathcal{O}_K$, which is the Dedekind zeta function ζ_K of the quadratic field K. ◊

Let us recall some properties of the Dedekind zeta function ζ_K. The latter is known [90] to factorise as

$$\zeta_K(s) \,=\, \zeta(s)\, L(s,\chi), \tag{3.5.7}$$

where $L(s,\chi)$ is the L-series of the non-trivial character $\chi = \chi_{d_K}$ of the quadratic field K. The latter is a totally multiplicative arithmetic function and thus given by $\chi_{d_K}(1)=1$ together with its values at the rational primes (that is, primes in $\mathbb{Z}\subset\mathbb{Q}$),

$$\chi_{d_K}(p) \,=\, \begin{cases} 0, & p \mid d_K, \\ \left(\frac{d_K}{p}\right), & 2\neq p \nmid d_K, \\ \left(\frac{d_K}{2}\right), & p=2 \nmid d_K. \end{cases}$$

Here, $\left(\frac{m}{p}\right)$ and $\left(\frac{m}{2}\right)$ denote the Legendre and the Kronecker symbol, respectively, the latter defined as

$$\left(\frac{m}{2}\right) \,=\, \begin{cases} 1, & m\equiv \pm 1\ (8), \\ -1, & m\equiv \pm 3\ (8), \\ 0, & m\equiv 0\ (2). \end{cases}$$

This permits a direct calculation of the zeta function via its Euler product, as the character $\chi(p)$ takes only the values 0, -1, or 1, depending on whether the rational prime p ramifies, is inert, or splits in the extension from $\mathbb{Q}$ to K. The general formula reads

$$\begin{aligned} \zeta_K(s) \,&=\, \prod_{p\in\mathbb{P}} \frac{1}{(1-p^{-s})(1-\chi(p)p^{-s})} \\ &=\, \prod_{\substack{p\in\mathbb{P}\\ \chi(p)=0}} \frac{1}{1-p^{-s}} \prod_{\substack{p\in\mathbb{P}\\ \chi(p)=-1}} \frac{1}{1-p^{-2s}} \prod_{\substack{p\in\mathbb{P}\\ \chi(p)=1}} \frac{1}{(1-p^{-s})^2}, \end{aligned} \tag{3.5.8}$$

where $\mathbb{P}$ denotes the set of rational primes.

The result on the generating functions now reads as follows.

Theorem 3.5.18 ([17, Prop. 5.2])**.** *Let K be any of the nine imaginary quadratic number fields of Lemma* 3.5.16*, with p_{ram} its ramified prime, which is the unique rational prime that divides d_K. The Dirichlet series generating function for the number of SSLs of $\mathcal{O}_K$ of a given index is $D_{\mathcal{O}_K}(s) = \zeta_K(s)$ with the Dedekind zeta function of K according to Eq.* (3.5.8)*.*

Moreover, the generating function for the primitive SSLs of $\mathcal{O}_K$ is

$$D^{\mathsf{pr}}_{\mathcal{O}_K}(s) \;=\; \frac{D_{\mathcal{O}_K}(s)}{\zeta(2s)} \;=\; (1+p_{\mathsf{ram}}^{-s}) \prod_{p \text{ splits}} \frac{1+p^{-s}}{1-p^{-s}},$$

where the product runs over all rational primes p that split in the extension to K. The same generating function also applies to any other planar lattice $\Gamma \in \mathrm{sim}(\mathcal{O}_K)$. □

In addition to the PIDs mentioned above, there are four additional (non-maximal) orders with class number 1, which we have summarised in Table 3.5.2. Their ideals are closely related to the ideals of their corresponding maximal orders. As a consequence, the generating functions $D_{\mathcal{O}}(s)$ and $D^{\mathsf{pr}}_{\mathcal{O}}(s)$ possess an Euler product. Their Euler factors are the same as those of the corresponding maximal order, except for the Euler factors corresponding to the primes that divide the *conductor* $f := [\mathcal{O}_K : \mathcal{O}]$. These special Euler factors can be calculated explicitly.

Theorem 3.5.19 ([17, Sec. 5.2])**.** *Let $\mathcal{O}$ be one of the four non-maximal orders of class number* 1 *in imaginary quadratic number fields as given in Table* 3.5.2*. The sublattice counting functions are multiplicative, which implies that their generating functions $D_{\mathcal{O}}(s)$ and $D^{\mathsf{pr}}_{\mathcal{O}}(s)$ have an Euler product expansion. In particular,*

$$D^{\mathsf{pr}}_{\mathbb{Z}[\mathrm{i}\sqrt{3}\,]}(s) \;=\; \Bigl(1+\frac{2}{4^s}\Bigr)\Bigl(1+\frac{1}{3^s}\Bigr) \prod_{p\equiv 1\,(3)} \frac{1+p^{-s}}{1-p^{-s}},$$

$$D^{\mathsf{pr}}_{\mathbb{Z}[2\,\mathrm{i}\,]}(s) \;=\; \Bigl(1+\frac{1}{4^s}+\frac{2}{8^s}\Bigr) \prod_{p\equiv 1\,(4)} \frac{1+p^{-s}}{1-p^{-s}},$$

$$D^{\mathsf{pr}}_{\mathbb{Z}[\frac{1}{2}(1+\mathrm{i}\,3\sqrt{3}\,)]}(s) \;=\; \Bigl(1+\frac{2}{9^s}+\frac{3}{27^s}\Bigr) \prod_{p\equiv 1\,(3)} \frac{1+p^{-s}}{1-p^{-s}},$$

$$D^{\mathsf{pr}}_{\mathbb{Z}[\mathrm{i}\sqrt{7}\,]}(s) \;=\; \Bigl(1-\frac{2}{2^s}+\frac{2}{4^s}\Bigr)\Bigl(1+\frac{1}{7^s}\Bigr) \prod_{p\equiv 1,2,4\,(7)} \frac{1+p^{-s}}{1-p^{-s}}.$$

TABLE 3.5.2. Basic data for the four non-maximal orders of class number 1 in imaginary quadratic number fields, labelled with their discriminant D; see Theorem 3.5.19 for details.

D	K	$\mathcal{O}$	norm form	$p \mid D$	conductor
-12	$\mathbb{Q}(\mathrm{i}\sqrt{3}\,)$	$\mathbb{Z}[\mathrm{i}\sqrt{3}\,]$	x^2+3y^2	$2,3$	2
-16	$\mathbb{Q}(\mathrm{i})$	$\mathbb{Z}[2\mathrm{i}]$	x^2+4y^2	2	2
-27	$\mathbb{Q}(\mathrm{i}\sqrt{3}\,)$	$\mathbb{Z}[\frac{1}{2}(1+\mathrm{i}3\sqrt{3}\,)]$	$x^2+xy+7y^2$	3	3
-28	$\mathbb{Q}(\mathrm{i}\sqrt{7}\,)$	$\mathbb{Z}[\mathrm{i}\sqrt{7}\,]$	x^2+7y^2	$2,7$	2

Again, the possible indices of the SSLs are precisely those positive integers that can be represented by the corresponding norm forms, which we have listed in Table 3.5.2. □

The situation is more involved for class numbers greater than 1, where the existence of non-principal ideals complicates the treatment. In general, the counting functions are no longer multiplicative, because a product of non-principal ideals may be principal. As a consequence, not much is known in these cases. However, there is still one situation that allows further treatment, namely when the discriminant D is one of Euler's *convenient numbers*, in which case the ideal class group is an Abelian 2-group. The latter implies that we have a natural binary grading on the ideals, depending on whether they are principal or not. If the order under investigation is still principal, one can derive the generating function from the zeta function; compare [17].

Example 3.5.20. Let us consider $\mathcal{O} = \mathbb{Z}[\mathrm{i}\sqrt{6}\,]$, where

$$D^{\mathsf{pr}}_{\mathbb{Z}[\mathrm{i}\sqrt{6}\,]}(s) \,=\, \prod_{p\equiv 1,7\,(24)} \frac{1+p^{-s}}{1-p^{-s}} \sum_{m=1}^{\infty} \frac{b(m)}{m^s}$$

with $b(1)=1$ and $b(m)=0$ if $p|m$ for some $p \equiv 1,7,13,17,19,23 \bmod 24$. If m is an integer of the form $m = 2^{\alpha}3^{\beta}\prod_{p\equiv 5,11\,(24)} p^{\ell_p}$ with $\alpha,\beta \in \{0,1\}$ and $\ell_p \in \mathbb{N}_0$, with only finitely many of them $\neq 0$, we have

$$b(m) \,=\, \bigl(1+(-1)^{\alpha+\beta+\sum \ell_p}\bigr)^{\mathrm{card}\{p>3\,|\,\ell_p\neq 0\}}.$$

Obviously, $D^{\mathsf{pr}}_{\mathbb{Z}[\mathrm{i}\sqrt{6}\,]}(s)$ possesses no Euler product representation. ◊

Example 3.5.21. As further cases, let us mention the generating functions for the primitive SSLs of $\mathcal{O} = \mathbb{Z}[3\mathrm{i}]$,

$$D^{\mathsf{pr}}_{\mathbb{Z}[3\mathrm{i}]}(s) \,=\, \sum_{\substack{m\geqslant 1\\ m\equiv 1\,(3)}} (1+9^s)\,\frac{a^{\mathsf{pr}}_{\square}(m)}{(9m)^s} \,+\, \sum_{\substack{m\geqslant 1\\ m\equiv 2\,(3)}} \frac{2\,a^{\mathsf{pr}}_{\square}(m)}{(9m)^s}, \tag{3.5.9}$$

and of $\mathcal{O} = \mathbb{Z}[5\mathrm{i}]$,

$$D^{\mathsf{pr}}_{\mathbb{Z}[5\,\mathrm{i}]}(s) \;=\; \sum_{\substack{m\geqslant 1\\ m\equiv \pm 1\,(5)}} (1+25^s)\,\frac{a^{\mathsf{pr}}_{\square}(m)}{(25m)^s} \;+\; \sum_{\substack{m\geqslant 1\\ m\equiv 0,\pm 2\,(5)}} \frac{2\,a^{\mathsf{pr}}_{\square}(m)}{(25m)^s}, \tag{3.5.10}$$

where $a^{\mathsf{pr}}_{\square}(m)$ is the number of primitive SSLs of index m of the square lattice; compare Section 3.3. ◊

Let us stay in two dimensions a little longer and discuss some $\mathbb{Z}$-modules with N-fold rotational symmetry. As this works the same way as for lattices, we include their discussion here, but see Section 3.6 for the general theory behind it. In particular, we consider the ring $\mathbb{Z}[\xi_n]$ of cyclotomic integers, where ξ_n is a primitive nth root of unity. If

$$\begin{aligned} n \;\in\; \{&3,4,5,7,8,9,11,12,13,15,16,17,19,20,21,24,\\ &25,27,28,32,33,35,36,40,44,45,48,60,84\}, \end{aligned} \tag{3.5.11}$$

the ring $\mathbb{Z}[\xi_n]$ is a PID, which means that the similar submodules are precisely the ideals of $\mathbb{Z}[\xi_n]$; compare [88, 7, AO1]. Using the terminology from above, this implies that $\mathbb{Z}[\xi_n]$ is its own multiplier ring. Note that $n = 3$ and $n = 4$ correspond to the hexagonal and the square lattice, respectively; compare [AO1, Ex. 2.15]. More generally, $\mathbb{Z}[\xi_n]$ is a $\mathbb{Z}$-module of rank $d = \phi(n)$, which is larger than 2 in the remaining cases; see [AO1, Rem. 3.7 and Ex. 2.16]. Here, ϕ denotes Euler's totient function. In particular, $\mathbb{Z}[\xi_n]$ has N-fold rotational symmetry, with $N = \mathrm{lcm}(n, 2)$.

As mentioned above, the similar submodules are precisely the non-trivial ideals of $\mathbb{Z}[\xi_n]$, which means that the generating function for the similar submodules of $\mathbb{Z}[\xi_n]$ is given by [7]

$$\Phi_{\mathbb{Z}[\xi_n]}(s) \;=\; \zeta_{\mathbb{Q}(\zeta_n)}(s) \;:=\; \sum_{\mathfrak{a}} \frac{1}{\mathrm{norm}(\mathfrak{a})^s}, \tag{3.5.12}$$

where the sum runs over all non-trivial ideals $\mathfrak{a}$ of $\mathbb{Z}[\xi_n]$ and

$$\mathrm{norm}(\mathfrak{a}) \;:=\; [\mathbb{Z}[\xi_n] : \mathfrak{a}]$$

denotes the norm of $\mathfrak{a}$. As $\mathbb{Z}[\xi_n]$ is a PID for all n from Eq. (3.5.11), the counting function for the ideals of fixed index is multiplicative. This, in turn, means that $\Phi_{\mathbb{Z}[\xi_n]}(s)$ has an Euler product expansion [7]

$$\Phi_{\mathbb{Z}[\xi_n]}(s) \;=\; \prod_{p\in\mathbb{P}} E_n(p^{-s}). \tag{3.5.13}$$

The Euler factors $E_n(p^{-s})$ are of the form

$$E_n(p^{-s}) \;=\; \frac{1}{(1-p^{-\ell s})^m} \;=\sum_{j=1}^{\infty} \binom{j+m-1}{m-1} \frac{1}{(p^s)^{\ell j}} \tag{3.5.14}$$

where m and ℓ are certain integers that depend on p and n. If p is coprime to n, then ℓ is the residue class degree of p, which is the smallest integer ℓ such that $p^\ell \equiv 1 \bmod n$, compare [88, Thm. 2.13] and [7]. The integer m is determined by $m\ell = \phi(n)$. If p divides n (p is a ramified prime in this case), we write $n = rp^t$, where p^t is the maximal power dividing n, so that r is the p-free part of n. The integers ℓ and m are now calculated by replacing n by r in the equations above, where ℓ is the smallest integer such that $p^\ell \equiv 1 \bmod r$ and $m\ell = \phi(r)$; compare the remarks after [88, Thm. 2.13] as well as [7]. Explicit values for m and ℓ, for all cases of Eq. (3.5.11), can be found in [7, Tables 1 and 2].

Example 3.5.22. Let us take a closer look at $\mathbb{Z}[\xi_5] = \mathbb{Z}[\xi_{10}]$. The only ramified prime is $5 = \varepsilon(1-\xi_5)^4$, where $\varepsilon = -\xi_5^2/\tau^2$ is a unit in $\mathbb{Z}[\xi_5]$. In terms of ideals, this means $(5) = (1-\xi_5)^4$. This gives $\ell = m = 1$ for $p = 5$. In addition, we get $\ell = 1$, $m = 4$ for $p \equiv 1 \bmod 5$, $\ell = 2$, $m = 2$ for $p \equiv -1 \bmod 5$, and $\ell = 4$, $m = 1$ for $p \equiv \pm 2 \bmod 5$. Thus, we obtain the generating function

$$\begin{aligned}\Phi_{\mathbb{Z}[\xi_5]}(s) &= \frac{1}{1-5^s} \prod_{p\equiv 1\,(5)} \frac{1}{(1-p^s)^4} \prod_{p\equiv -1\,(5)} \frac{1}{(1-p^{2s})^2} \prod_{p\equiv \pm 2\,(5)} \frac{1}{1-p^{4s}} \\ &= 1 + \frac{1}{5^s} + \frac{4}{11^s} + \frac{1}{16^s} + \frac{1}{25^s} + \frac{4}{31^s} + \frac{4}{41^s} + \frac{4}{55^s} + \frac{4}{61^s} \\ &\quad + \frac{4}{71^s} + \frac{1}{80^s} + \frac{1}{81^s} + \frac{4}{101^s} + \frac{10}{121^s} + \frac{1}{125^s} + \frac{4}{131^s} + \dots\end{aligned}$$

for this case. ◊

3.5.3. Higher dimensions

Let us continue with lattices in higher dimensions. We concentrate on *rational* lattices[4] here, that is, on lattices Γ for which the inner products satisfy $\langle x|y\rangle \in \mathbb{Q}$ for all $x, y \in \Gamma$. For all scaling factors $\alpha \in \mathrm{Scal}_\Gamma(R)$, one then has $\alpha^2 \in \mathbb{Q}$. By an application of Lemma 3.5.5, we may conclude that $\alpha^2 \in \mathbb{Z}$. Moreover, one obtains the stronger condition $\alpha \in \mathbb{Z}$ in odd dimensions, again by Lemma 3.5.5. This gives the following result.

Fact 3.5.23. *For a rational lattice $\Gamma \subset \mathbb{R}^d$ with d odd, the possible indices of SSLs are exactly the integers of the form n^d with $n \in \mathbb{N}$.* □

Thus, the question for the possible indices is answered in this case, and we may proceed with lattices in even dimension, say $d = 2k$. As $\alpha^2 \in \mathbb{Z}$, the possible indices of SSLs are all of the form c^k with $c \in \mathbb{N}$. For an important class of $2k$-dimensional lattices, an answer was given by Conway, Rains and

[4]More generally, one calls a lattice Γ rational if there exists an $\alpha > 0$ such that $\langle x|y\rangle \in \mathbb{Q}$ for all $x, y \in \alpha\Gamma$. In this section, we only use the more restrictive definition.

Sloane in [25]. Let $\mathbb{Z}_p$ denote the p-adic integers [AO1, Ex. 2.10] and define the Hilbert symbol $(a,b)_p$ as

$$(a,b)_p = \begin{cases} 1, & \text{if } z^2 = ax^2 + by^2 \text{ has a non-zero solution in } \mathbb{Z}_p, \\ -1, & \text{otherwise.} \end{cases}$$

Their result can now be formulated as follows.[5]

Theorem 3.5.24 ([25, Thm. 1])**.** *Let $\Gamma \subset \mathbb{R}^{2k}$ be a rational lattice. An SSL of index c^k can only exist if the condition*

$$\big(c, (-1)^k \det(\Gamma)\big)_p = 1$$

is satisfied for all primes p that divide $2c\det(\Gamma)$. If Γ is unigeneric and (r)-maximal for some $r \in \mathbb{Q}$, then this condition is also sufficient. □

Here, (r)-*maximal* means that Γ is maximal with respect to the property that $\langle x|x\rangle \in r\mathbb{Z}$ for all $x \in \Gamma$. It is *unigeneric* if it is unique in its genus. Recall that the genus of a rational quadratic form is the set of quadratic forms that are $\mathbb{R}$-equivalent and $\mathbb{Z}_p$-equivalent for any prime p; compare [24]. In other words, a rational quadratic form Q is unigeneric if and only if any other quadratic form Q' that is $\mathbb{Z}_p$-equivalent to Q for any prime p as well as $\mathbb{R}$-equivalent to Q then also is $\mathbb{Z}$-equivalent to Q. The correspondence between lattices and quadratic forms then transfers these notions to lattices.

Example 3.5.25. Theorem 3.5.24 can now be applied to several lattices [25], which are all unigeneric and (1)- or (2)-maximal.

(1) The root lattice A_4 has SSLs of index c^2 for $c = \mathrm{nr}(z) = zz'$ only, where $z \in \mathbb{Z}[\tau]$ with $\tau = \big(1+\sqrt{5}\big)/2$ and z' is the algebraic conjugate of z. Consequently, rational primes $p \equiv \pm 2 \bmod 5$ appear to even powers in c.

(2) The hypercubic lattice $\mathbb{Z}^6$ has SSLs of index c^3 for $c = \mathrm{nr}(z) = |z|^2$ only, where $z \in \mathbb{Z}[\mathrm{i}]$. Here, rational primes $p \equiv 3 \bmod 4$ appear to even powers in c.

(3) The root lattice E_6 has SSLs of index c^3 for $c = \mathrm{nr}(z) = |z|^2$ only, where $z \in \mathbb{Z}[(1+\mathrm{i}\sqrt{3})/2]$. Rational primes $p \equiv 2 \bmod 3$ thus appear to even powers in c. ◊

[5] The authors formulate their results on sublattices in terms of the norm $c = \alpha^2$ of a similarity $\sigma = \alpha R$. We prefer to employ the index $n = [\Gamma : \alpha R\Gamma] = \alpha^d = c^{d/2}$ instead. The use of the norm c is natural for rational lattices, as it is always an integer in these cases. However, it is less meaningful for general lattices, where the natural quantity is the index n. To keep our notation consistent, we stick to the formulation in terms of the index here, which explains the additional exponent $\frac{d}{2}$ in our formulation.

Further details for the root lattice A_4 will be discussed below. Another consequence of Theorem 3.5.24 is the following result, where the notation for the lattices is taken from [26, Ch. 4].

Corollary 3.5.26 ([25, Thm. 3])**.** *The lattices $\mathbb{Z}^{4m}$, D_{4m} and D_{4m}^{+} possess SSLs of index c^{2m} for all $c \in \mathbb{N}$. Similarly, the lattices E_8, K_{12}, the Barnes–Wall lattice BW_{16} and the Leech lattice Λ_{24} possess SSLs of index c^4, c^6, c^8 and c^{12}, respectively, for all $c \in \mathbb{N}$.* □

3.5.4. The root lattice A_4

For the lattice A_4, we can go further and count the SSLs of a given index explicitly. Usually, A_4 is embedded in $\mathbb{R}^5$ as a lattice plane, but this is inconvenient for our purposes and we prefer to look at it in $\mathbb{R}^4$, since we want to exploit a useful parametrisation by quaternions.

Consider the lattice $L \subset \mathbb{R}^4$ that is spanned by the four vectors

$$(1,0,0,0),\ \tfrac{1}{2}(-1,1,1,1),\ (0,-1,0,0),\ \tfrac{1}{2}(0,1,\tau-1,-\tau), \tag{3.5.15}$$

with $\tau = \bigl(1+\sqrt{5}\bigr)/2$ as before. Then, L is similar to A_4, with the scale reduced by a factor $\sqrt{2}$; compare [AO1, Ex. 3.3] or [15]. This way, we have $L \subset \mathbb{I}$, where $\mathbb{I}$ denotes the icosian ring; see [AO1, Ex. 2.19] and references therein.

Let us begin by recalling some properties of L. Both L and $\mathbb{I}$ are invariant under quaternionic conjugation, so $L = \overline{L}$ and $\mathbb{I} = \overline{\mathbb{I}}$, but neither of them is invariant under algebraic conjugation $\tau \mapsto \tau'$. Combining the algebraic conjugation with a permutation of the last two (quaternionic) components yields another involution, $x \mapsto \widetilde{x} := (x_0', x_1', x_3', x_2')$, which is an involution of the second kind in the terminology of [59] and was called the *twist map* in [15, 16]. Note that $L = \widetilde{L}$ is invariant under the twist map, which, in addition, is an anti-automorphism of $\mathbb{I}$. In other words, the twist map has the following properties.

Fact 3.5.27 ([15, Lemma 1])**.** *For any $x, y \in \mathbb{I}$ and $\alpha \in \mathbb{Q}(\tau)$, one has*

(1) $\widetilde{x+y} = \widetilde{x} + \widetilde{y}$ *and* $\widetilde{\alpha x} = \alpha' \widetilde{x}$;
(2) $\widetilde{xy} = \widetilde{y}\widetilde{x}$ *and* $\widetilde{\widetilde{x}} = x$;
(3) $\widetilde{\overline{x}} = \overline{\widetilde{x}}$ *and, for $x \neq 0$,* $(\widetilde{x})^{-1} = \widetilde{x^{-1}}$. □

The twist map is the key to our analysis as it gives us a convenient parametrisation of the similarity rotations — and later also the coincidence rotations. Furthermore, it provides us with the following characterisation [15, Prop. 1] of the lattice L as a subset of $\mathbb{I}$,

$$L = \{x \in \mathbb{I} \mid x = \widetilde{x}\}. \tag{3.5.16}$$

By Cayley's parametrisation (3.4.2), we know that any rotation in $\mathbb{R}^4$ can be written as $R(p,q)x = \frac{1}{|pq|}px\bar{q}$. Using the properties of the twist map and the characterisation of L from above, we immediately see that $qL\widetilde{q} \subseteq L$ is a similar sublattice of L for any $q \in \mathbb{I}$. In fact, any SSL of L is of the form $\alpha qL\widetilde{q} \subseteq L$, with $q \in \mathbb{I}$ and $\alpha \in \mathbb{Q}(\tau)$; see [15, Cor. 1].

In order to classify the SSLs, it is convenient to introduce a suitable primitivity notion on $\mathbb{I}$. A quaternion $q \in \mathbb{I}$ is called $\mathbb{I}$-*primitive* (or primitive for short) if $\alpha q \in \mathbb{I}$ with $\alpha \in \mathbb{Q}(\tau)$ implies $\alpha \in \mathbb{Z}[\tau]$. Equivalently, $q \in \mathbb{I}$ is $\mathbb{I}$-primitive if the $\mathbb{I}$-content of q,

$$\mathrm{cont}_{\mathbb{I}}(q) \,:=\, \mathrm{lcm}\big\{\alpha \in \mathbb{Z}[\tau] \setminus \{0\} \mid q \in \alpha\mathbb{I}\big\},$$

is a unit in $\mathbb{Z}[\tau]$. Note that the notion of an lcm makes sense because $\mathbb{Z}[\tau]$ is a Euclidean domain. Of course, $\mathrm{cont}_{\mathbb{I}}(q)$ is defined only up to a unit in $\mathbb{Z}[\tau]$. We can now fully characterise the SSLs as follows.

Lemma 3.5.28 ([15, Cor. 2])**.** *The primitive SSLs of L are precisely the sublattices of the form $qL\widetilde{q}$, where $q \in \mathbb{I}$ is $\mathbb{I}$-primitive. Consequently, the SSLs of L are precisely the sublattices of the form $nqL\widetilde{q}$ with $n \in \mathbb{N}$ and $q \in \mathbb{I}$ primitive.* □

As we also want to determine the number of distinct SSLs of a given index, we need to ensure that we do not count the same SSL twice. In general, different quaternions may generate the same SSL, so we need a criterion to determine whether two SSLs $qL\widetilde{q}$ and $pL\widetilde{p}$ are equal. One first observes that $L = qL\widetilde{q}$ holds for an $\mathbb{I}$-primitive quaternion q if and only if $q \in \mathbb{I}^\times$, where $\mathbb{I}^\times$ is the unit group in $\mathbb{I}$; see [AO1, Ex. 2.19] for an explicit description and [69, 70] for further background. From here, one can infer the following result.

Fact 3.5.29 ([15, Lemma 5])**.** *For $\mathbb{I}$-primitive quaternions $p, q \in \mathbb{I}$, one has $pL\widetilde{p} = qL\widetilde{q}$ if and only if $p\mathbb{I} = q\mathbb{I}$.* □

This fact reduces the problem of counting SSLs of L to the problem of counting primitive right ideals of $\mathbb{I}$. Here, we call a right ideal $q\mathbb{I}$ primitive if q is $\mathbb{I}$-primitive.

The index of a primitive SSL can be determined by an explicit calculation. We mention that $|\widetilde{q}|^2 = (|q|^2)'$ holds for any $q \in \mathbb{I}$. Recall from [AO1, Ex. 2.14] that the *norm* of an element $\alpha \in \mathbb{Q}(\tau)$ is defined as

$$\mathrm{nr}(\alpha) \,=\, \alpha\alpha'.$$

The index of a primitive SSL $qL\widetilde{q}$ then satisfies $[L : qL\widetilde{q}] = \mathrm{nr}(|q|^4)$. As $q\mathbb{I}$ has index $\mathrm{nr}(|q|^4)$ in $\mathbb{I}$ as well, we get the following result.

Lemma 3.5.30 ([15, Prop. 4])**.** *There is a bijective correspondence between the primitive right ideals of $\mathbb{I}$ and the primitive SSLs of L, given by $q\mathbb{I} \leftrightarrow qL\widetilde{q}$. Moreover, one has*

$$\big[\mathbb{I} : q\mathbb{I}\big] \;=\; \mathrm{nr}\big(|q|^4\big) \;=\; \big[L : qL\widetilde{q}\big],$$

which means that the bijection preserves the index. □

As a consequence, all possible indices are squares of integers of the form $k^2 + k\ell - \ell^2 = \mathrm{nr}(k + \ell\tau)$. In fact, all these indices are realised [15, 25]. As the number of right ideals of $\mathbb{I}$ of a given index is well known, we can deduce the numbers $b_{A_4}(m)$ and $b^{\mathsf{pr}}_{A_4}(m)$ of SSLs and primitive SSLs of index m, respectively. This can efficiently be done by employing the corresponding Dirichlet series generating functions. To do so, we first recall the Dirichlet character

$$\chi_5(n) = \begin{cases} 0, & \text{if } n \equiv 0 \ (5), \\ 1, & \text{if } n \equiv \pm 1 \ (5), \\ -1, & \text{if } n \equiv \pm 2 \ (5). \end{cases}$$

Its corresponding L-series, $L(s, \chi_5) = \sum_{n=1}^{\infty} \chi_5(n) n^{-s}$, defines (via analytic continuation) an entire function on the complex plane. The Dedekind zeta function of $K = \mathbb{Q}(\tau)$ is given by $\zeta_K(s) = \zeta(s)L(s, \chi_5)$, which is a meromorphic function. Likewise, the zeta function $\zeta_{\mathbb{I}}$ of the icosian ring [86, 11], which counts the right (or left) ideals of $\mathbb{I}$, is meromorphic in the entire complex plane and reads

$$\zeta_{\mathbb{I}}(s) \;=\; \zeta_K(2s)\,\zeta_K(2s-1). \tag{3.5.17}$$

As the Dirichlet series of the two-sided ideals is given by $\zeta_K(4s)$, one obtains the zeta function $\zeta^{\mathsf{pr}}_{\mathbb{I}}$ of the primitive ideals [11] as

$$\zeta^{\mathsf{pr}}_{\mathbb{I}}(s) \;=\; \frac{\zeta_K(2s)\,\zeta_K(2s-1)}{\zeta_K(4s)}. \tag{3.5.18}$$

This leads to the following result.

Theorem 3.5.31 ([15, Thm. 1])**.** *The Dirichlet series generating functions for the numbers $b_{A_4}(n)$ and $b^{\mathsf{pr}}_{A_4}(n)$ of SSLs and primitive SSLs of the root lattice A_4 of a given index are*

$$\Phi_{A_4}(s) \;=\; \sum_{n\in\mathbb{N}} \frac{b_{A_4}(n)}{n^s} \;=\; \zeta(4s)\,\frac{\zeta_{\mathbb{I}}(s)}{\zeta_K(4s)} \;=\; \frac{\zeta_K(2s)\,\zeta_K(2s-1)}{L(4s,\chi_5)}$$

and

$$\Phi^{\mathsf{pr}}_{A_4}(s) \;=\; \sum_{n\in\mathbb{N}} \frac{b^{\mathsf{pr}}_{A_4}(n)}{n^s} \;=\; \zeta^{\mathsf{pr}}_{\mathbb{I}}(s) \;=\; \frac{\zeta_K(2s)\,\zeta_K(2s-1)}{\zeta_K(4s)}.$$ □

Both generating functions from Theorem 3.5.31 possess Euler products, which read

$$\begin{aligned}\Phi_{A_4}(s) \;&=\; \frac{1}{(1-5^{-2s})(1-5^{1-2s})} \prod_{p\equiv\pm1(5)} \frac{1+p^{-2s}}{(1-p^{-2s})(1-p^{1-2s})^2} \\ &\quad\times \prod_{p\equiv\pm2(5)} \frac{1+p^{-4s}}{(1-p^{-4s})(1-p^{2-4s})}\end{aligned} \tag{3.5.19}$$

and

$$\Phi^{\mathsf{pr}}_{A_4}(s) \;=\; \frac{1+5^{-2s}}{1-5^{1-2s}} \prod_{p\equiv\pm1(5)} \frac{(1+p^{-2s})^2}{(1-p^{1-2s})^2} \prod_{p\equiv\pm2(5)} \frac{1+p^{-4s}}{1-p^{2-4s}}. \tag{3.5.20}$$

From these identities, we can obtain explicit expressions for $b_{A_4}(n)$ and $b^{\mathsf{pr}}_{A_4}(n)$, which are multiplicative arithmetic functions. Thus, they are determined by their values at prime powers. As $b_{A_4}(p^{2r+1}) = b^{\mathsf{pr}}_{A_4}(p^{2r+1}) = 0$, we only need to state their values for primes at even powers $\geqslant 2$. The result is [15]

$$b_{A_4}(p^{2r}) = \begin{cases} \frac{5^{r+1}-1}{4}, & \text{if } p = 5, \\ \frac{(r+1)(p^2-1)p^r-2(p^{r+1}-1)}{(p-1)^2}, & \text{if } p \equiv \pm1\,(5), \\ \frac{p^{r+2}+p^r-2}{p^2-1}, & \text{if } p \equiv \pm2\,(5) \text{ and } r \text{ even}, \\ 0, & \text{if } p \equiv \pm2\,(5) \text{ and } r \text{ odd}, \end{cases}$$

and

$$b^{\mathsf{pr}}_{A_4}(p^{2r}) = \begin{cases} 6\cdot 5^{r-1}, & \text{if } p = 5, \\ (r+1)p^r + 2rp^{r-1} + (r-1)p^{r-2}, & \text{if } p \equiv \pm1\,(5), \\ p^r + p^{r-2}, & \text{if } p \equiv \pm2\,(5) \text{ and } r \text{ even}, \\ 0, & \text{if } p \equiv \pm2\,(5) \text{ and } r \text{ odd}. \end{cases}$$

It follows from these formulas that all possible indices are not only realised for some SSL, but even realised for some *primitive* SSL. In fact, it will turn out that the majority of SSLs of a given index are primitive. This can be illustrated by comparing the first few terms of Φ_{A_4} and $\Phi^{\mathsf{pr}}_{A_4}$,

$$\Phi_{A_4}(s) \;=\; 1 + \frac{6}{4^{2s}} + \frac{6}{5^{2s}} + \frac{11}{9^{2s}} + \frac{24}{11^{2s}} + \frac{26}{16^{2s}} + \frac{40}{19^{2s}} + \frac{36}{20^{2s}} + \frac{31}{25^{2s}} + \cdots,$$

$$\Phi^{\mathsf{pr}}_{A_4}(s) \;=\; 1 + \frac{5}{4^{2s}} + \frac{6}{5^{2s}} + \frac{10}{9^{2s}} + \frac{24}{11^{2s}} + \frac{20}{16^{2s}} + \frac{40}{19^{2s}} + \frac{30}{20^{2s}} + \frac{30}{25^{2s}} + \cdots.$$

The explicit form of the generating functions $\Phi_{A_4}(s)$ and $\Phi^{\mathsf{pr}}_{A_4}$ allows us to calculate the asymptotic behaviour of $b_{A_4}(n)$ and $b^{\mathsf{pr}}_{A_4}(n)$. The result reads as follows.

Corollary 3.5.32 ([15, Sec. 4])**.** *The asymptotic growth of the summatory function of* $b_{A_4}(n)$ *is*

$$\sum_{m \leqslant x} b_{A_4}(m) \sim \frac{\rho}{2} x, \quad \text{as } x \to \infty,$$

where ρ *is given by*

$$\rho = \frac{\zeta_K(2) L(1, \chi_5)}{L(4, \chi_5)} = \frac{1}{2}\sqrt{5}\log(\tau) \approx 0.538011.$$

The asymptotic growth for $b^{\mathsf{pr}}_{A_4}(n)$ *is also linear, now with*

$$\rho^{\mathsf{pr}} = \frac{\zeta_K(2) L(1, \chi_5)}{\zeta(4) L(4, \chi_5)} = \frac{45}{\pi^4}\sqrt{5}\log(\tau) \approx 0.497089. \qquad \square$$

SKETCH OF PROOF. We apply again Theorem 3.4.1, this time to the generating functions given in Theorem 3.5.31. The fact that both Dirichlet series are meromorphic functions, which are analytic in the half-plane $\{\mathrm{Re}(s) > 1\}$ and have the proper behaviour on the line $\{\mathrm{Re}(s) = 1\}$, implies the linear growth. The explicit calculations for $\sum_{m \leqslant x} b_{A_4}(m)$ are similar[6] to those from [15, Sec. 4, p. 1402]. The case of the primitive SSLs is analogous, and just gives an additional factor $\frac{1}{\zeta(4)}$. $\square$

3.5.5. Hypercubic lattices in $\mathbb{R}^4$

There are, up to similarity, two hypercubic lattices in 4 dimensions, namely the primitive hypercubic lattice $\mathbb{Z}^4$ and the centred hypercubic lattice D_4; compare [26] and [AO1, Ex. 3.2]. The latter is similar to its dual lattice D_4^*, which we identify with the Hurwitz ring $\mathbb{J}$.

Recall that any rotation in 4 dimensions can be parametrised by a pair of quaternions; compare Section 3.4.1. It turns out that any similarity rotation of $\Gamma \in \{D_4^*, \mathbb{Z}^4\}$ can be parametrised by a pair (p, q) of Hurwitz quaternions. Moreover, any SSL of Γ is of the form $p\Gamma\bar{q}$, where we can choose p to be odd and primitive; compare [11, Rem. 1 and Lemma 2]. With this convention, in the case of $\Gamma = D_4^* = \mathbb{J}$, p and q are unique up to multiplication by a unit of $\mathbb{J}$ from the right [11, Prop. 3]. Hence, counting SSLs of D_4^* is equivalent to counting right ideals of $\mathbb{J}$.

The situation is slightly more complicated for $\mathbb{Z}^4$, as its symmetry is lower. As a consequence, there may be three distinct (but, of course, congruent) SSLs of $\mathbb{Z}^4$ that correspond to a single SSL of $\mathbb{J}$. This only happens if the index of the SSL is even. We thus obtain the following result for the

[6]Note that a different definition for the counting function was applied in [15]. There, the function $f(m) = b_{A_4}(m^2)$ was discussed, which makes sense as $b_{A_4}(n)$ is non-zero only for squares. Correspondingly, the asymptotics for $f(m)$ are given by $\sum_{m \leqslant x} f(m) \sim \frac{\rho}{2} x^2$ as $x \to \infty$.

generating functions of the SSLs, where we make use of the zeta function of $\mathbb{J}$, which reads [11, 86, 76]

$$\zeta_{\mathbb{J}}(s) \,=\sum_{I\subseteq\mathbb{J}} \frac{1}{[\mathbb{J}:I]^s} \;=\; (1-2^{1-2s})\,\zeta(2s)\,\zeta(2s-1). \tag{3.5.21}$$

Theorem 3.5.33 ([11, Thm. 2])**.** *The possible indices of similar sublattices of hypercubic lattices in $\mathbb{R}^4$ are precisely the squares of rational integers. The number of distinct SSLs of a given index is a multiplicative arithmetic function. For the case of $\mathbb{J} = D_4^*$, the corresponding Dirichlet series generating function $\Phi_{\mathbb{J}}$ reads*

$$\Phi_{\mathbb{J}}(s) \;=\; \frac{\bigl(\zeta_{\mathbb{J}}(s)\bigr)^2}{(1+4^{-s})\,\zeta(4s)} \;=\; \frac{\bigl(1-2^{1-2s}\bigr)^2}{1+4^{-s}}\,\frac{\bigl(\zeta(2s)\,\zeta(2s-1)\bigr)^2}{\zeta(4s)}.$$

The same function also applies to the lattice D_4, while we obtain

$$\Phi_{\mathbb{Z}^4}(s) \;=\; \Bigl(1+\frac{2}{4^s}\Bigr)\,\Phi_{\mathbb{J}}(s)$$

for the primitive hypercubic lattice $\mathbb{Z}^4$. □

From the generating functions of Theorem 3.5.33, we can extract the corresponding counting functions $b_{\mathbb{J}}(m)$ and $b_{\mathbb{Z}^4}(m)$. We formulate them in terms of the function

$$g(n,r) \;=\; (r+1)\,n^r + 2\,\frac{1-(r+1)n^r+rn^{r+1}}{(n-1)^2} \tag{3.5.22}$$

for integers $r \geqslant 0$ and $n > 1$.

Corollary 3.5.34 ([11, Cor. 1])**.** *The arithmetic functions $b_{\mathbb{J}}(m)$ and $b_{\mathbb{Z}^4}(m)$ are multiplicative. They are non-zero if and only if m is a square, and are then determined by*

$$b_{\mathbb{J}}(p^{2r}) \;=\; \begin{cases} 1, & \text{if } p=2,\\ g(p,r), & \text{if } p \text{ is an odd prime,}\end{cases}$$

for all $r \geqslant 0$, and by $b_{\mathbb{Z}^4}(m) = (2+(-1)^m)\,b_{\mathbb{J}}(m)$. □

The first few terms of $\Phi_{\mathbb{J}}(s)$ read

$$\begin{aligned}\Phi_{\mathbb{J}}(s) \;=\; 1 &+ \frac{1}{4^s}+\frac{8}{9^s}+\frac{1}{16^s}+\frac{12}{25^s}+\frac{8}{36^s}+\frac{16}{49^s}+\frac{1}{64^s}+\frac{41}{81^s}+\frac{12}{100^s}\\ &+\frac{24}{121^s}+\frac{8}{144^s}+\frac{28}{169^s}+\frac{16}{196^s}+\frac{96}{225^s}+\frac{1}{256^s}+\frac{36}{289^s}+\cdots,\end{aligned}$$

which corresponds to sequence A045771 in [84].

Corollary 3.5.35 ([11, Cor. 2])**.** *The asymptotic growth of the summatory function* $\sum_{m\leqslant x} b_\Gamma(m)$ *is given by*[7]

$$\sum_{m\leqslant x} b_\Gamma(m) \;\sim\; C_\Gamma\, x \log(x)$$

as $x \to \infty$*, where the constant* C_Γ *is given by*

$$C_\Gamma \;=\; \operatorname{res}_{s=1}\big((s-1)\Phi_\Gamma(s)\big) \;=\; \begin{cases} \frac{1}{8}, & \text{for } \Gamma = \mathbb{J}, \\ \frac{3}{16}, & \text{for } \Gamma = \mathbb{Z}^4. \end{cases} \qquad \square$$

Finally, let us comment on the primitive SSLs. A pair (p, q) of Hurwitz quaternions generates a primitive SSL of $\mathbb{J}$ if and only if both p and q are $\mathbb{J}$-primitive and at least one of them is odd.

In this case, the denominator of the corresponding rotation is given by

$$\operatorname{den}_{\mathbb{J}}(R(p,q)) \;=\; |pq|. \tag{3.5.23}$$

For $\mathbb{Z}^4$, a pair of $\mathbb{J}$-primitive quaternions does not necessarily generate an SSL of $\mathbb{Z}^4$. This only works if $pq \in \mathbb{Z}^4$. Consequently, primitive SSLs are either of the form $p\mathbb{Z}^4\bar{q}$ or $2p\mathbb{Z}^4\bar{q}$, depending on whether $pq \in \mathbb{Z}^4$ or not. Correspondingly, the denominator for $\mathbb{Z}^4$ reads

$$\operatorname{den}_{\mathbb{Z}^4}(R(p,q)) \;=\; \begin{cases} |pq|, & \text{if } pq \in \mathbb{Z}^4, \\ 2|pq|, & \text{if } pq \notin \mathbb{Z}^4. \end{cases} \tag{3.5.24}$$

As a consequence, we have $\Phi^{\mathsf{pr}}_\Gamma(s) = \Phi_\Gamma(s)/\zeta(4s)$ for $\Gamma \in \{\mathbb{J}, \mathbb{Z}^4\}$. Finally, this yields the asymptotic behaviour

$$\sum_{m\leqslant x} b^{\mathsf{pr}}_\Gamma(m) \;\sim\; C^{\mathsf{pr}}_\Gamma\, x \log(x) \quad \text{with} \quad C^{\mathsf{pr}}_\Gamma \;=\; \begin{cases} \frac{45}{4\pi^4}, & \text{for } \Gamma = \mathbb{J}, \\ \frac{135}{8\pi^4}, & \text{for } \Gamma = \mathbb{Z}^4. \end{cases}$$

3.6. Similar submodules

Here, we are interested in $\mathbb{Z}$-modules as generalisations of lattices. As such, they are mainly considered as *geometric* (as opposed to algebraic) objects. Let us thus begin with a definition of the geometric setting.

Definition 3.6.1. A $\mathbb{Z}$-module M of rank n is called (properly) *embedded* in $\mathbb{R}^d$ when $M \subset \mathbb{R}^d$ and when there is a $\mathbb{Z}$-basis $\{b_1, \dots, b_n\}$ of M whose $\mathbb{R}$-span is $\mathbb{R}^d$.

---

[7] Note that in [11] the asymptotics of the counting function $f_\Gamma(m) = b_\Gamma(m^2)$ instead of $b_\Gamma(m)$ are discussed; compare Footnote 6. Correspondingly, the asymptotics for $f_\Gamma(m)$ are given by $\sum_{m\leqslant x} f_\Gamma(m) \sim 2C_\Gamma\, x^2 \log(x)$ as $x \to \infty$.

In particular, this requires that $n \geqslant d$, where n is the *rank* of M and d may be called its *embedding dimension*. A lattice is an embedded module with $n = d$. An important class of embedded modules is given by what we call $\mathcal{S}$-lattices.

Definition 3.6.2. Let $\mathcal{S} \subset \mathbb{R}$ be a ring with identity that is also a finitely generated, free $\mathbb{Z}$-module. Then, we call an embedded $\mathbb{Z}$-module $M \subset \mathbb{R}^d$ an *$\mathcal{S}$-lattice*, if there exist d linearly independent vectors $b_i \in \mathbb{R}^d$ such that M is the $\mathcal{S}$-span of $\{b_1, \ldots, b_d\}$, so $M = \langle b_1, \ldots, b_d \rangle_{\mathcal{S}}$.

We call a $\mathbb{Z}$-module $M' \subseteq M$ a (full) *submodule* of M if M' and M have the same rank.[8] This implies that M' and M also have the same embedding dimension, wherefore the index $[M : M']$ is finite.

Just as for lattices, we define the more general notion of commensurate modules.

Definition 3.6.3. Two (properly embedded) $\mathbb{Z}$-modules $M_1, M_2 \subset \mathbb{R}^d$ are called *commensurate*, which is denoted by $M_1 \sim M_2$, if their intersection $M_1 \cap M_2$ has finite index in both M_1 and M_2.

In our terminology, this means that M_1 and M_2 are commensurate if and only if $M_1 \cap M_2$ is a submodule of both M_1 and M_2 in our above sense. This implies that M_1 and M_2 can only be commensurate if they have the same rank. Once we know that two embedded modules in $\mathbb{R}^d$ have the same rank, the situation becomes easier as we can characterise commensurateness in several ways [97], which we recall here.

Lemma 3.6.4. *Let $M_1, M_2 \subseteq \mathbb{R}^d$ be two properly embedded $\mathbb{Z}$-modules of rank k. Then, the following statements are equivalent.*

(1) *M_1 and M_2 are commensurate.*
(2) *$M_1 \cap M_2$ has finite index in both M_1 and M_2.*
(3) *$M_1 \cap M_2$ has finite index in M_1 or in M_2.*
(4) *There exist (positive) integers m_1 and m_2 such that $m_1 M_1 \subseteq M_2$ and $m_2 M_2 \subseteq M_1$.*
(5) *There exists an integer m such that $mM_1 \subseteq M_2$ or $mM_2 \subseteq M_1$.*
(6) *$M_1 \cap M_2$ has rank k.* □

To continue, two properly embedded modules M_1 and M_2 are called *similar*, $M_1 \overset{\mathsf{s}}{\sim} M_2$, if there exists a similarity transformation between them. Clearly, similarity of modules is an equivalence relation.

[8] More generally, one calls any $\mathbb{Z}$-module $M' \subseteq M$ a submodule of M regardless of its rank, but we do not need this more general notion in our context.

Definition 3.6.5. A similarity transformation that maps a module $M \subset \mathbb{R}^d$ onto a submodule of M is called a *similarity transformation of* M. A submodule $M' \subseteq M$ is called a *similar submodule* (SSM) of M if $M' \overset{\mathsf{s}}{\sim} M$.

We proceed as before and consider coincidence isometries and scaling factors separately. We first define

$$\mathrm{OS}(M) := \{R \in \mathrm{O}(d,\mathbb{R}) \mid \exists \alpha \in \mathbb{R}_+ \text{ such that } \alpha RM \subseteq M\} \tag{3.6.1}$$

whose elements are called *similarity isometries* of M. Similarly, we use

$$\mathrm{SOS}(M) := \mathrm{OS}(M) \cap \mathrm{SO}(d,\mathbb{R}) \tag{3.6.2}$$

to denote the set of similarity rotations. The following results are immediate generalisations of the corresponding results for lattices in Fact 3.5.1 and Lemma 3.5.2.

Fact 3.6.6. $\mathrm{OS}(M)$ *and* $\mathrm{SOS}(M)$ *are subgroups of* $\mathrm{O}(d,\mathbb{R})$. *Further, if* M *and* $M' = \alpha RM$ *are similar modules which are both embedded in* $\mathbb{R}^d$, *we have*

$$\mathrm{OS}(M') \;=\; R\,\mathrm{OS}(M)\,R^{-1}. \qquad \square$$

Next, we consider the scaling factors. We first define

$$\begin{aligned} \mathrm{Scal}_M(R) &:= \{\alpha \in \mathbb{R} \mid \alpha RM \subseteq M\} \quad \text{and} \\ \mathrm{scal}_M(R) &:= \{\alpha \in \mathbb{R} \mid \alpha RM \sim M\}. \end{aligned} \tag{3.6.3}$$

Again, we have allowed negative values for the scaling factors here to ensure that $\mathrm{Scal}_M(R)$ is a $\mathbb{Z}$-module. This creates no problem because $-M = M$. However, the situation is more complicated than in the case of lattices, as there are significantly fewer restrictions on the scaling factors here.

Note that $\mathrm{Scal}_M(R)$ is non-empty for all R as $0 \in \mathrm{Scal}_M(R)$, but it is non-trivial only if $R \in \mathrm{OS}(M)$, as we have the following generalisation of Fact 3.5.3.

Fact 3.6.7 ([97, p. 14])**.** *Let* $M \subset \mathbb{R}^d$ *be an embedded* $\mathbb{Z}$*-module and consider* $R \in \mathrm{O}(d,\mathbb{R})$. *Then, the following properties are equivalent.*

(1) $\mathrm{Scal}_M(R) \neq \{0\}$*;*
(2) $\mathrm{scal}_M(R) \neq \varnothing$*;*
(3) $R \in \mathrm{OS}(M)$. $\square$

As a first consequence, we mention a result on the possible values of $\mathrm{Scal}_M(\mathbb{1})$. Recall that $[x]$ denotes the largest integer $n \leqslant x$.

Theorem 3.6.8 ([97, Thm. 2.1.6 and Cor. 2.1.7])**.** *Let* $M \subset \mathbb{R}^d$ *be an embedded* $\mathbb{Z}$*-module of rank* k. *Then,* $\mathrm{Scal}_M(\mathbb{1})$ *is a ring with unit all elements of which are algebraic integers. Moreover,* $\mathrm{Scal}_M(\mathbb{1})$ *is a finitely generated, free* $\mathbb{Z}$*-module, whose rank is a divisor of* k *and is at most* $\left[\frac{k}{d}\right]$.

Furthermore, $\mathrm{scal}_M(\mathbb{1}) \cup \{0\}$ *is the field of fractions of* $\mathrm{Scal}_M(\mathbb{1})$. □

For $\mathcal{S}$-lattices, we can immediately determine $\mathrm{Scal}_M(\mathbb{1})$ and $\mathrm{scal}_M(\mathbb{1})$.

Fact 3.6.9. *If* M *is an* $\mathcal{S}$*-lattice, then* $\mathrm{Scal}_M(\mathbb{1}) = \mathcal{S}$ *and* $\mathrm{scal}_M(\mathbb{1}) \cup \{0\}$ *is the field of fractions of* $\mathcal{S}$.

Proof. Since $\mathcal{S}$ is a ring and M is the $\mathcal{S}$-span of d linearly independent vectors $b_i \in \mathbb{R}^d$, we have $\mathcal{S} \subseteq \mathrm{Scal}_M(\mathbb{1})$. On the other hand, the linear independence of the b_i guarantees $\mathrm{Scal}_M(\mathbb{1})b_1 \subseteq M \cap \mathbb{R}b_1 = \mathcal{S}b_1$, whence we have the reverse inclusion $\mathrm{Scal}_M(\mathbb{1}) \subseteq \mathcal{S}$. The second part now follows immediately from Theorem 3.6.8; compare also [43, Remark 3.11]. □

For general similarity isometries R, we have the following result.

Theorem 3.6.10 ([97, Thm. 2.1.9])**.** *Let* $M \subset \mathbb{R}^d$ *be an embedded* $\mathbb{Z}$*-module. Then, for any* $R \in \mathrm{OS}(M)$, $\mathrm{Scal}_M(R)$ *is a finitely generated, free* $\mathbb{Z}$*-module. Moreover,* $\beta\,\mathrm{Scal}_M(R) \subseteq \mathrm{Scal}_M(R)$ *for any* $\beta \in \mathrm{Scal}_M(\mathbb{1})$*, and* $\mathrm{Scal}_M(R)$ *is thus also a finitely generated* $\mathrm{Scal}_M(\mathbb{1})$*-module.* □

Observe that $\mathrm{Scal}_M(R)$ is generally not a free $\mathrm{Scal}_M(\mathbb{1})$-module, unless $\mathrm{Scal}_M(\mathbb{1})$ is a PID; see [97, p. 15] for an example.

For lattices, Lemma 3.5.5 asserted that $\alpha^d \in \mathbb{Z}$ for all $\alpha \in \mathrm{Scal}_\Gamma(R)$. The corresponding result for embedded modules reads as follows.

Theorem 3.6.11 ([97, Thm. 2.1.10])**.** *As before, let* $M \subset \mathbb{R}^d$ *be an embedded* $\mathbb{Z}$*-module of finite rank. Then, any* $\alpha \in \mathrm{Scal}_M(R)$ *is an algebraic integer. If* M *has rank* $k = 1$*, one always has* $\mathrm{Scal}_M(R) = \mathbb{Z}$*, so* α *is a rational integer in this case. If* $k \geqslant 2$*, the degree of* α *is at most* $k(k-1)$. □

The set $\{\mathrm{scal}_M(R) \mid R \in \mathrm{OS}(M)\}$ has again a group structure, under the multiplication defined by

$$\mathrm{scal}_M(R)\,\mathrm{scal}_M(S) := \{\alpha\beta \mid \alpha \in \mathrm{scal}_M(R), \beta \in \mathrm{scal}_M(S)\}.$$

We have the following generalisation of Lemma 3.5.8.

Theorem 3.6.12 ([97, Lemmas 2.1.11 and 2.1.12 and Thm. 2.1.12])**.** *Let* $M \subset \mathbb{R}^d$ *be an embedded* $\mathbb{Z}$*-module. Then, one has the following properties.*

(1) *For any* $R, S \in \mathrm{OS}(M)$*, we have the product relation*

$$\mathrm{scal}_M(R)\,\mathrm{scal}_M(S) = \mathrm{scal}_M(RS)$$

together with $\mathrm{scal}_M(R^{-1})\,\mathrm{scal}_M(R) = \mathrm{scal}_M(\mathbb{1})$.

(2) $\{\mathrm{scal}_M(R) \mid R \in \mathrm{OS}(M)\}$ *is an Abelian group. Its neutral element is* $\mathrm{scal}_M(\mathbb{1})$*, and the inverse of* $\mathrm{scal}_M(R)$ *is* $\mathrm{scal}_M(R^{-1})$.

(3) $\{\mathrm{scal}_M(R) \mid R \in \mathrm{OS}(M)\}$ *is isomorphic to a multiplicative subgroup of* $\mathbb{R}_+/(\mathrm{scal}_M(\mathbb{1}) \cap \mathbb{R}_+)$.

(4) *There exists a natural homomorphism*

$$\phi\colon \mathrm{OS}(M) \longrightarrow \{\mathrm{scal}_M(R) \mid R \in \mathrm{OS}(M)\}$$

via $R \mapsto \mathrm{scal}_M(R)$. □

In fact, this theorem will be the key to establish the connection between CSMs and SSMs in Section 3.7.6.

As $\mathrm{Scal}_M(R)$ need not be a PID, we cannot characterise it by a denominator as in Section 3.5. This makes it more difficult to establish a connection between the sets $\mathrm{Scal}_M(R)$ for related modules. Nevertheless, there are some results.

Lemma 3.6.13 ([97, Lemmas 2.2.1 and 2.2.2])**.** *If M and N are commensurate modules, one has* $\mathrm{OS}(M) = \mathrm{OS}(N)$ *and* $\mathrm{scal}_N(R) = \mathrm{scal}_M(R)$ *for any* $R \in \mathrm{OS}(M) = \mathrm{OS}(N)$. □

For $\mathrm{Scal}_M(R)$, a weaker result applies.

Theorem 3.6.14 ([97, Thm. 2.2.3])**.** *Let N be a submodule of M of index m. Then,* $m\,\mathrm{Scal}_M(R) \subseteq \mathrm{Scal}_N(R) \subseteq \frac{1}{m}\,\mathrm{Scal}_M(R)$. □

Above, we have already considered some examples of planar modules in Section 3.5.2. We conclude our discussion of SSMs with an important example in $\mathbb{R}^4$.

3.6.1. The icosian ring

We already met the icosian ring $\mathbb{I}$ in connection with the lattice A_4, where it was used as a tool to determine the SSLs of A_4. But it is also interesting to classify the SSMs of $\mathbb{I}$ itself.

Actually, the way to determine the SSMs is completely analogous to the case of $\mathbb{J}$ in the previous section, which is related to the fact that both $\mathbb{J}$ and $\mathbb{I}$ are maximal orders in their corresponding quaternion algebras; compare [76]. Although $\mathbb{I}$ is not a lattice but a $\mathbb{Z}$-module in $\mathbb{R}^4$, all steps can be easily generalised for $\mathbb{I}$, as the latter can be viewed as a $\mathbb{Z}[\tau]$-module of rank 4 (or a $\mathbb{Z}[\tau]$-lattice in our above terminology) that is properly embedded in $\mathbb{R}^4$. Moreover, any quaternion in $\mathbb{I}$ has a norm which lies in $\mathbb{Z}[\tau]$. Thus, the zeta function of the number field $K = \mathbb{Q}(\tau)$ comes into play again, and we can express the generating function of the SSMs in terms of $\zeta_{\mathbb{I}}(s)$, which we know from Eq. (3.5.17).

Theorem 3.6.15 ([11, Thm. 3])**.** *The possible indices of similar submodules of the icosian ring are precisely the squares of rational integers that can be represented by the quadratic form $x^2 + xy - y^2$. The number of SSMs of a given index is a multiplicative arithmetic function, whose Dirichlet series*

generating function $\Phi_{\mathbb{I}}$ *reads*

$$\Phi_{\mathbb{I}}(s) \,=\, \frac{\bigl(\zeta_{\mathbb{I}}(s)\bigr)^2}{\zeta_K(4s)} \,=\, \frac{\bigl(\zeta_K(2s)\,\zeta_K(2s-1)\bigr)^2}{\zeta_K(4s)}$$

with $K = \mathbb{Q}(\tau)$. □

This theorem allows us to infer the corresponding counting function $b_{\mathbb{I}}(m)$. Using the function $g(n,r)$ defined previously in Eq. (3.5.22), we obtain the following explicit result.

Corollary 3.6.16 ([11, Cor. 3])**.** *The arithmetic function* $b_{\mathbb{I}}(m)$ *is multiplicative and vanishes unless* m *is a square. It is completely determined by specifying* $b_{\mathbb{I}}(p^{2r})$ *for all rational primes* p *and all* $r \geqslant 0$*. With the function* g *of Eq.* (3.5.22)*, one has*

$$b_{\mathbb{I}}(p^{2r}) \,=\, \begin{cases} g(5,r), & \text{if } p = 5, \\ 0, & \text{if } p \equiv \pm 2\,(5) \text{ and } r \text{ is odd}, \\ g(p^2, \frac{r}{2}), & \text{if } p \equiv \pm 2\,(5) \text{ and } r \text{ is even}, \\ \sum_{\ell=0}^{r} g(p,\ell)g(p,r-\ell), & \text{if } p \equiv \pm 1\,(5). \end{cases}$$ □

The first few terms of $\Phi_{\mathbb{I}}(s)$ read

$$\begin{aligned}\Phi_{\mathbb{I}}(s) \,=\, 1 &+ \frac{10}{4^{2s}} + \frac{12}{5^{2s}} + \frac{20}{9^{2s}} + \frac{48}{11^{2s}} + \frac{66}{16^{2s}} + \frac{80}{19^{2s}} + \frac{120}{20^{2s}} + \frac{97}{25^{2s}} \\ &+ \frac{120}{29^{2s}} + \frac{128}{31^{2s}} + \frac{200}{36^{2s}} + \frac{168}{41^{2s}} + \frac{480}{44^{2s}} + \frac{240}{45^{2s}} + \cdots\end{aligned}$$

Along the same lines as before, we can evaluate the asymptotic behaviour.

Corollary 3.6.17 ([11, Cor. 4])**.** *The asymptotic growth of the summatory function* $\sum_{m \leqslant x} b_{\mathbb{I}}(m)$ *is given by*[9]

$$\sum_{m \leqslant x} b_{\mathbb{I}}(m) \,\sim\, \frac{3\log(\tau)^2}{5\sqrt{5}}\, x\log(x) \,\approx\, 0.062135\, x\log(x)$$

as $x \to \infty$. □

Let us now turn our attention to the related problem of coincidence site lattices. It is less common in the mathematical literature, due to its origin in crystallography. As we shall see, it is technically more involved and thus less developed from a structural point of view. Nevertheless, its consideration is completely natural and intrinsically connected with the SSL problem, as we shall see later on.

[9] Compare Footnotes 6 and 7 on pages 104 and 106, respectively.

3.7. Coincidence site lattices and modules

3.7.1. Basic facts

Let us return to the CSLs, which we have introduced in Definition 3.2.5. To parallel our approach to the SSLs, we introduce the set

$$\mathrm{OC}(\varGamma) := \{R \in \mathrm{O}(d,\mathbb{R}) \mid \varGamma \sim R\varGamma\}, \tag{3.7.1}$$

where $\varGamma \subset \mathbb{R}^d$ is a (given) lattice. Likewise, we use the notation

$$\mathrm{SOC}(\varGamma) := \{R \in \mathrm{OC}(\varGamma) \mid \det(R) = 1\} \tag{3.7.2}$$

for the set of all orientation-preserving coincidence isometries, which are also known as coincidence rotations. Let us mention that the groups $\mathrm{OC}(\varGamma)$ and $\mathrm{SOC}(\varGamma)$ can be interpreted as *commensurator groups* of the lattice $\varGamma$; compare [12].

Fact 3.7.1 ([4, Thm. 2.1])**.** *The sets* $\mathrm{OC}(\varGamma)$ *and* $\mathrm{SOC}(\varGamma)$ *are subgroups of* $\mathrm{O}(d,\mathbb{R})$. □

Note that $\mathrm{OC}(\varGamma)$ contains the symmetry group $\mathrm{O}(\varGamma)$ of $\varGamma$ as a subgroup. Indeed, $\mathrm{O}(\varGamma)$ is precisely the group of all coincidence isometries of index $\varSigma_{\varGamma}(R) = [\varGamma : \varGamma(R)] = 1$; compare Definition 3.2.5.

One certainly expects connections between lattices that are closely related. Here, one has the following elementary result.

Lemma 3.7.2 ([4, Cor. 2.1 and Lemma 2.6])**.** *Commensurate lattices have the same* OC*-groups. In particular, all sublattices of a lattice* $\varGamma$ *have the same group of coincidence isometries.* □

We have seen earlier in Lemma 3.5.2 that similar lattices have conjugate OS-groups. A corresponding result for coincidence isometries exists as well.

Lemma 3.7.3 ([4, Lemma 2.5])**.** *Similar lattices have conjugate* OC*-groups. In particular, for any* $0 \neq \alpha \in \mathbb{R}$ *and any* $R \in \mathrm{O}(d,\mathbb{R})$*, one has*

$$\mathrm{OC}(\alpha R\varGamma) \;=\; R\,\mathrm{OC}(\varGamma)\,R^{-1},$$

together with $\varSigma_{\alpha R\varGamma}(S) = \varSigma_{\varGamma}(R^{-1}SR)$. □

Unsurprisingly, there is also a close connection between a lattice and its dual lattice; compare [4].

Lemma 3.7.4. *Let* $\varGamma^*$ *be the dual lattice of a lattice* $\varGamma \subseteq \mathbb{R}^d$*. Then,* $\mathrm{OC}(\varGamma^*) = \mathrm{OC}(\varGamma)$ *and* $\varSigma_{\varGamma^*}(R) = \varSigma_{\varGamma}(R)$ *for all* $R \in \mathrm{OC}(\varGamma)$.

Proof. As two lattices are commensurate if and only if their duals are commensurate, we have $\varGamma^* \sim R\varGamma^*$ if and only if $\varGamma \sim R\varGamma$, where one needs the

relation $(R\varGamma)^* = R\varGamma^*$. By definition, this implies $\mathrm{OC}(\varGamma^*) = \mathrm{OC}(\varGamma)$. Now,

$$[\varGamma^* : \varGamma^*(R)] \,=\, [\varGamma^* : (\varGamma + R\varGamma)^*] \,=\, [\varGamma + R\varGamma : \varGamma] \,=\, [\varGamma : \varGamma(R)],$$

which proves the claim. □

An interesting observation is that the coincidence indices of a coincidence isometry and its inverse are the same. This fact can be proved by geometric arguments [4] involving the dual lattice, which we will repeat here.

Lemma 3.7.5. *Let $\varGamma \subseteq \mathbb{R}^d$ be a lattice. For any $R \in \mathrm{OC}(\varGamma)$, one has*

$$\varSigma_{\varGamma}(R) \,=\, \varSigma_{\varGamma}(R^{-1}).$$

Proof. The key is the fact that $[\varGamma : \varGamma(R)]$ can be interpreted geometrically: It is the ratio of the volumes of fundamental cells of $\varGamma(R)$ and $\varGamma$, which is independent of the particular choice of the latter. As isometries preserve the volume, we have

$$\begin{aligned}\varSigma_{\varGamma}(R) \,&=\, [\varGamma : \varGamma(R)] \,=\, [R\varGamma : \varGamma(R)] \,=\, [R\varGamma : \varGamma \cap R\varGamma] \\ &=\, [\varGamma : R^{-1}\varGamma \cap \varGamma] \,=\, \varSigma_{\varGamma}(R^{-1}),\end{aligned}$$

which completes the argument. □

As $\mathrm{OC}(\varGamma)$ is a group, it is natural to ask whether there is a connection between the indices $\varSigma_{\varGamma}(R_1)$, $\varSigma_{\varGamma}(R_2)$ and $\varSigma_{\varGamma}(R_1R_2)$ for $R_1, R_2 \in \mathrm{OC}(\varGamma)$. Although no general formula exists which expresses one of them in terms of the other two, we have the following results.

Theorem 3.7.6 ([95], [97, Lemma 3.4.3 and Thm. 3.4.4])**.** *For any lattice $\varGamma \subset \mathbb{R}^d$ and for any $R_1, R_2 \in \mathrm{OC}(\varGamma)$, one has the following relations.*

(1) *$\varSigma_{\varGamma}(R_1R_2)$ divides $\varSigma_{\varGamma}(R_1)\varSigma_{\varGamma}(R_2)$.*
(2) *$\varSigma_{\varGamma}(R_1R_2) = \varSigma_{\varGamma}(R_1)\varSigma_{\varGamma}(R_2)$ whenever $\varSigma_{\varGamma}(R_1)$ and $\varSigma_{\varGamma}(R_2)$ are coprime.* □

Remark 3.7.7. In particular, one has $\varSigma_{\varGamma}(RS) = \varSigma_{\varGamma}(R)$ if $\varSigma_{\varGamma}(S) = 1$, or in other words, if $S \in \mathrm{O}(\varGamma)$, which means that S is a symmetry operation of $\varGamma$. Actually, if $S \in \mathrm{O}(\varGamma)$, one even has $\varGamma(RS) = \varGamma(R)$. This motivates us to call two coincidence isometries R and R' *symmetry related* if there exists an $S \in \mathrm{O}(\varGamma)$ such that $R' = RS$. Thus, symmetry-related coincidence isometries generate the same CSL, but the converse is not true in general; see Example 3.7.16 below for an instance of two coincidence isometries that are not symmetry related but generate the same CSL. ◊

Remark 3.7.8. One of the quantities we are after is the set of possible coincidence indices. In line with [12], we call this set,

$$\sigma(\varGamma) \,=\, \varSigma(\mathrm{OC}(\varGamma)) \,=\, \{\varSigma_{\varGamma}(R) \mid R \in \mathrm{OC}(\varGamma)\},$$

the *coincidence spectrum* of Γ. Sometimes, we call it the ordinary or simple coincidence spectrum to distinguish it from the multiple coincidence spectrum, which we define later; compare Section 3.7.2. Likewise, $\Sigma(\mathrm{SOC}(\Gamma)) = \{\Sigma_\Gamma(R) \mid R \in \mathrm{SOC}(\Gamma)\}$ is the subset of indices of the coincidence rotations. Clearly, we have $\Sigma(\mathrm{SOC}(\Gamma)) \subseteq \Sigma(\mathrm{OC}(\Gamma))$ in general, but in many cases we have $\Sigma(\mathrm{SOC}(\Gamma)) = \Sigma(\mathrm{OC}(\Gamma))$. By Remark 3.7.7, $\Sigma(\mathrm{SOC}(\Gamma)) = \Sigma(\mathrm{OC}(\Gamma))$ whenever an orientation-reversing isometry exists in $\mathrm{O}(\Gamma)$, but this is only a sufficient condition and by no means a necessary one. ◊

It is not uncommon that one needs to relate the coincidence structure of a lattice to that of various sublattices. Let us consider some consequences on the coincidence indices.

Lemma 3.7.9. *Let Λ be a sublattice of $\Gamma \subseteq \mathbb{R}^d$ of index m. Then, $\Sigma_\Lambda(R)$ divides $m\Sigma_\Gamma(R)$ and $\Sigma_\Gamma(R)$ divides $m\Sigma_\Lambda(R)$.*

Proof. As $\Lambda(R) \subseteq \Gamma(R) \subseteq \Gamma$, the coincidence index $\Sigma_\Gamma(R)$ divides

$$[\Gamma : \Lambda(R)] = [\Gamma : \Lambda]\,[\Lambda : \Lambda(R)] = m\Sigma_\Lambda(R),$$

which proves the second claim.

The first claim can be proved by applying Lemma 3.7.4. It is well known that $\Lambda \subseteq \Gamma$ implies $\Gamma^* \subseteq \Lambda^*$. Since $\Sigma_\Gamma(R) = \Sigma_{\Gamma^*}(R)$ by Lemma 3.7.4, for any lattice Γ, the result now follows immediately from the first part of the proof. □

Lemma 3.7.9 provides us with some useful bounds on the coincidence indices of a sublattice. In certain cases, we can even get sharper bounds [64, 97]. As an example, we mention the following result, which is a special case of [97, Thm. 3.1.10] or [64, Thm. 2.2] (with $u = 1$ in the notation used there).

Lemma 3.7.10. *Let Λ be a sublattice of Γ of index m, and let $R \in \mathrm{OC}(\Gamma)$ be such that $\Lambda \cap R(t + \Lambda) = \varnothing$ for all $t \in \Gamma \setminus \Lambda$. Then, $\Sigma_\Lambda(R)$ divides $\Sigma_\Gamma(R)$.* □

Note that this result is the basis of the concept of *colour coincidences*; compare [64, 62, 66].

Remark 3.7.11. Lemma 3.7.10 is only useful in practice if it is reasonably easy to check the condition $\Lambda \cap R(t + \Lambda) = \varnothing$ for all $t \in \Gamma \setminus \Lambda$. This is possible if the points of Λ and $\Gamma \setminus \Lambda$ lie on different shells, that is, if the sets $\big\{|x| \,\big|\, x \in \Lambda\big\}$ and $\big\{|x| \,\big|\, x \in \Gamma \setminus \Lambda\big\}$ are disjoint. This way, one can show that the three classes of cubic lattices have the same coincidence indices, as we shall see later in Section 3.9. ◊

Remark 3.7.12. The shelling structure of lattices is a well-studied problem. It leads to Θ-series, which are nicely summarised in [26, Sec. 2.2.3]. The problem has also been investigated for embedded $\mathbb{Z}$-modules such as rings of cyclotomic integers in the plane [6], for the icosian ring in 4-space [69], or for $\mathbb{Z}$-modules in 3-space with icosahedral symmetry [89]. Also, Penrose-type tilings have been considered, where the notion of an *averaged shelling* was introduced [9]. In the latter case, an interpretation of the results in a wider setting is still missing. ◊

3.7.2. Multiple coincidences

We can generalise our considerations on CSLs by looking at intersections of more than two commensurate lattices. The analogous step for modules will briefly be discussed in Section 3.7.5. This problem is interesting for various reasons. On the one hand, these intersections naturally occur in the discussion of the counting functions for CSLs; see Section 3.7.4 and [95]. On the other hand, they are important in crystallography in connection with multiple junctions [39, 40, 41]. Another interesting application arises in the theory of lattice quantisers where one usually deals with rather complex lattices. There, one hopes to simplify the problem by representing a complex lattice as the intersection of simpler lattices [33, 83].

In fact, intersections of more than two isometric commensurate copies of a lattice have already been discussed in [8, 94, 13, 97]. Let us first recall the corresponding definitions.

Definition 3.7.13. Let $\varGamma \subseteq \mathbb{R}^d$ be a lattice and assume $R_i \in \mathrm{OC}(\varGamma)$, with $i \in \{1, \ldots m\}$. The lattice

$$\varGamma(R_1, \ldots, R_m) := \varGamma \cap R_1\varGamma \cap \ldots \cap R_m\varGamma = \varGamma(R_1) \cap \ldots \cap \varGamma(R_m)$$

is then called a *multiple* CSL (MCSL) of order m. Its index in $\varGamma$ is denoted by $\varSigma(R_1, \ldots, R_m)$.

In order to distinguish CSLs of the type $\varGamma(R) = \varGamma \cap R\varGamma$ from multiple CSLs, we will occasionally use the term simple or ordinary CSL for $\varGamma(R)$.

Note that $\varSigma(R_1, \ldots, R_m)$ is finite since $\varGamma(R_1, \ldots, R_m)$ is a finite intersection of mutually commensurate lattices [4]. In particular, an immediate consequence of the second isomorphism theorem for groups is the following result.

Lemma 3.7.14 ([97, Lemma 3.3.1])**.** *For $R_1, R_2 \in \mathrm{OC}(\varGamma)$, one has*

$$\varSigma(R_1, R_2) = \frac{\varSigma(R_1)\,\varSigma(R_2)}{\varSigma_+(R_1, R_2)},$$

where $\Sigma_+(R_1, R_2)$ is the index of the direct sum $\Gamma_+(R_1, R_2) = \Gamma(R_1)+\Gamma(R_2)$ in the lattice Γ. □

More generally, one has the following relation.

Lemma 3.7.15 ([97, Lemma 3.3.2])**.** *For any $R_i \in \mathrm{OC}(\Gamma)$,*

$$\Sigma(R_1, \ldots, R_m) \;=\; \frac{\Sigma(R_1, \ldots, R_{m-1})\, \Sigma(R_m)}{\Sigma_+(R_1, \ldots, R_{m-1}; R_m)},$$

where $\Sigma_+(R_1, \ldots, R_{m-1}; R_m)$ is the index of

$$\Gamma_+(R_1, \ldots, R_{m-1}; R_m) \;=\; \Gamma(R_1, \ldots, R_{m-1}) + \Gamma(R_m)$$

in Γ. In particular, $\Sigma(R_1, \ldots, R_m)$ divides $\Sigma(R_1) \cdot \ldots \cdot \Sigma(R_m)$. □

This result allows us to infer some basic properties of the coincidence spectrum. Recall from Remark 3.7.8 that the simple coincidence spectrum was defined as $\sigma(\Gamma) = \{\Sigma_\Gamma(R) \mid R \in \mathrm{OC}(\Gamma)\}$. Likewise, we introduce the *multiple coincidence spectrum* as the set

$$\sigma_\infty(\Gamma) = \{\Sigma(R_1, \ldots, R_m) \mid R_i \in \mathrm{OC}(\Gamma), m \in \mathbb{N}\}.$$

Clearly, we have

$$\sigma(\Gamma) \;\subseteq\; \sigma_\infty(\Gamma) \;\subseteq\; \widehat{\sigma}(\Gamma), \tag{3.7.3}$$

where $\widehat{\sigma}(\Gamma)$ is the set of all positive integers that divide an integer from the (multiplicative) semigroup generated by $\sigma(\Gamma)$. We shall come back to this relation and possible consequences at the end of Section 3.12.2.

3.7.3. MCSLs and monotiles

In [AO1, Sec. 5.7.7], the SCD monotile due to Schmitt, Conway and Danzer for $\mathbb{R}^3$ is discussed. This convex tile, together with translated and rotated copies (but no reflected copies), allows to form periodic two-dimensional layers L, which can only be stacked vertically by rotating the layers by a fixed irrational rotation R. In particular, any tiling $\mathcal{T}$ of $\mathbb{R}^d$ obtained this way must have the form

$$\mathcal{T} \;=\; \bigcup_{m\in\mathbb{Z}} (mc + R^m L), \tag{3.7.4}$$

where c is a suitable vector orthogonal to the plane of the layer L; compare [AO1, Eq. (5.7)] and [32, 5]. As $R^n \neq \mathbb{1}$ for any $n \in \mathbb{Z} \setminus \{0\}$, any resulting tiling of $\mathbb{R}^d$ is aperiodic.

Let us analyse this construction in some more detail, in terms of MCSLs. Let L be one fixed layer of an SCD tiling. If Γ is the group of translations that leaves L invariant, then the stack of $n+1$ layers $\mathcal{T} = \bigcup_{m=0}^{n}(mc + R^m L)$ is invariant under the MCSL $\Gamma_n := \Gamma \cap R\Gamma \cap \ldots \cap R^n\Gamma$, with $\Gamma_0 = \Gamma$.

As $\bigcap_{n\in\mathbb{N}_0} \varGamma_n = \{0\}$, the tiling is aperiodic; compare [AO1, Lemma 5.8 and Rem. 5.12].

If we pursue these ideas further, we can construct monotiles in all odd dimensions $2m+1 \geqslant 3$. Let us start with a lattice $\varGamma \in \mathbb{R}^d$ for $d = 2m$ and assume that $\varGamma$ has a coincidence rotation R such that $R^n \neq \mathbb{1}$ for any $n \in \mathbb{Z} \setminus \{0\}$. We choose a unit cell U (possibly convex or a parallelohedron, with suitable markers) of the CSL $\varGamma \cap R\varGamma$ such that no lattice point of $\varGamma$ or $R\varGamma$ is on the boundary. We can always choose U in such a way that it tiles $\mathbb{R}^d$ only periodically, with $\varGamma$ as the corresponding lattice of periods. We define a prototile T in $\mathbb{R}^{d+1}$ as $U \times [0,1]$ and add markings on the bottom and the top of T as follows. On the bottom, we mark each lattice point of $\varGamma$ that is contained in U (to avoid any complication, we choose some mark without any symmetry) and on top we mark the lattice points of $R\varGamma$ (with the same marks just rotated by R). This guarantees that we can stack these layers of tiles vertically only by rotating them by R. Hence, the only tilings we can get are tilings of the form (3.7.4), with L replaced by $\varGamma$.

As $R^n \neq \mathbb{1}$ for any $n \in \mathbb{Z} \setminus \{0\}$, the tiling is not periodic in the remaining (transversal) direction. To exclude any periodicity in a direction parallel to the layers, we need $\bigcap_{n\in\mathbb{N}_0} \varGamma_n = \{0\}$. Such an R exists for the square lattice. In fact, each coincidence rotation R that is not a symmetry of the square lattice has this property. Likewise, $\mathbb{Z}^{2m}$ has infinitely many coincidence rotations R that satisfy $\bigcap_{n\in\mathbb{N}_0} \varGamma_n = \{0\}$. In particular, we may choose R as the direct product of two-dimensional coincidence rotations, each of which fails to be a symmetry of the square lattice.

However, note that, although all these tilings are aperiodic, they are not *strongly aperiodic*, as there is still a skew rotation symmetry left, which means that the symmetry group contains a subgroup isomorphic to $\mathbb{Z}$; compare [AO1, Def. 5.22]. In this sense, also the original SCD tiling is aperiodic, but not strongly aperiodic. To the best of our knowlegde, no strongly aperiodic monotile in 3-space is known.

With this restriction, the above construction establishes the existence of monotiles in odd dimensions. For even dimensions, the analogous construction fails, as the corresponding lattice then has odd dimension and any coincidence rotation of it leaves at least one lattice direction invariant. Whether monotiles exist in even dimensions is still an open problem. Only in dimension $d = 2$, a monotile for the Euclidean plane (with next-to-nearest neighbour local rules) was discovered by Joan Taylor; see [AO1, Sec. 5.7.6] and references therein for a more detailed account of the tiling, its properties (due to Socolar and Taylor) and predecessors (due to Penrose).

3.7.4. Counting functions

As sketched in Section 3.3, we are interested in several enumeration problems. In particular, for a given index, we are after the number of coincidence isometries and the number of CSLs. For a fixed lattice $\varGamma$, we shall denote the number of CSLs of a given index n by $c_{\varGamma}(n)$. As the same CSL can be generated by several coincidence isometries, it is not useful to deal with the total number of coincidence isometries directly, but it is more convenient to use a properly normalised counting function instead.

If S is a symmetry operation of $\varGamma$, we have $\varGamma(RS) = \varGamma(R)$ for any coincidence isometry R. This means that the number of coincidence isometries with a given index is a multiple of $\mathrm{card}(\mathrm{O}(\varGamma))$, where $\mathrm{O}(\varGamma)$ is the symmetry group of $\varGamma$. Thus, we prefer to deal with the function $c^{\mathsf{iso}}_{\varGamma}(n)$, which counts the coincidence isometries modulo the symmetry group. Then, the number of coincidence isometries of a given index n is given by $\mathrm{card}(\mathrm{O}(\varGamma))\, c^{\mathsf{iso}}_{\varGamma}(n)$. Likewise, we define $c^{\mathsf{rot}}_{\varGamma}(n)$ for all coincidence rotations, now counted modulo $\mathrm{SO}(\varGamma) = \mathrm{O}(\varGamma) \cap \mathrm{SO}(d)$. This guarantees $c^{\mathsf{iso}}_{\varGamma}(1) = c^{\mathsf{rot}}_{\varGamma}(1) = c_{\varGamma}(1)$.

Let us mention that $c^{\mathsf{rot}}_{\varGamma}(n) = c^{\mathsf{iso}}_{\varGamma}(n)$ holds whenever there exists an orientation-reversing symmetry operation. In particular, $c^{\mathsf{rot}}_{\varGamma}(n) = c^{\mathsf{iso}}_{\varGamma}(n)$ holds for every lattice $\varGamma$ in odd dimensions.

Recall from Remark 3.7.7 that two coincidence isometries R and R' are called *symmetry related*, if there exists a symmetry operation $S \in \mathrm{O}(\varGamma)$ such that $R' = RS$. As symmetry-related coincidence isometries generate the same CSL, it follows that $c^{\mathsf{iso}}_{\varGamma}(n)$ is an upper bound for $c_{\varGamma}(n)$. However, these two numbers differ in general, as non-symmetry-related coincidence isometries may still generate the same CSL.

Example 3.7.16. As an example for differing counting functions for lattices versus isometries, we consider the rectangular lattice $\varGamma = \mathbb{Z}[\mathrm{i}\sqrt{3}] \subset \mathbb{R}^2$, which is a sublattice of the hexagonal lattice $\varLambda = \mathbb{Z}[\omega]$ with $\omega = \frac{1+\mathrm{i}\sqrt{3}}{2}$. Then, one has the inclusions $2\varLambda \subset \varGamma \subset \varLambda$ with indices $[\varLambda : \varGamma] = [\varGamma : 2\varLambda] = 2$. As ω^k with $k \not\equiv 0 \bmod 3$ is a symmetry operation for $\varLambda$ but not for $\varGamma$, we infer $\varSigma_{\varGamma}(\omega^k) > 1 = \varSigma_{\varLambda}(\omega^k)$ for $k \in \{1, 2\}$. It follows from Lemma 3.7.9 that one in fact has $\varSigma_{\varGamma}(\omega^k) = 2 = [\varGamma : 2\varLambda]$. Together with $\varGamma(\omega^k) \supseteq 2\varLambda$, this gives $\varGamma(\omega^k) = 2\varLambda$ for $k \in \{1, 2\}$. As ω and ω^2 fail to be symmetry related, this implies $c^{\mathsf{iso}}_{\varGamma}(2) = c^{\mathsf{rot}}_{\varGamma}(2) > c_{\varGamma}(2)$. In fact, a more detailed analysis yields $c^{\mathsf{rot}}_{\varGamma}(2) = 2 > 1 = c_{\varGamma}(2)$.

This example can easily be generalised as follows. Whenever one has a lattice $\varLambda \subset \varGamma$ such that the index $[\varGamma : \varLambda] = p$ is a prime and such that $\mathrm{O}(\varGamma) \subset \mathrm{O}(\varLambda)$ with $[\mathrm{O}(\varLambda) : \mathrm{O}(\varGamma)] \geqslant 3$, one can infer $c^{\mathsf{iso}}_{\varGamma}(p) > c_{\varGamma}(p)$ by analogous arguments. Moreover, if p is not in the coincidence spectrum of $\varLambda$,

one can even show that

$$c_{\varGamma}^{\mathsf{iso}}(p) \,=\, [\mathrm{O}(\varLambda) : \mathrm{O}(\varGamma)] - 1 \,>\, 1 \,=\, c_{\varGamma}(p).$$

This follows from $\varSigma_{\varGamma}(R) = p$ together with the observation that $\varGamma(R) = \varLambda$ for any $R \in \mathrm{O}(\varLambda) \setminus \mathrm{O}(\varGamma)$. $\Diamond$

In several important examples, all these counting functions are multiplicative, which suggests the use of generating functions of Dirichlet series type to determine their asymptotic growth rate, as we have done in several examples so far. In general, however, the counting functions fail to be multiplicative, though we have the following weaker result.

Theorem 3.7.17 ([95, 97]). *The arithmetic function $c_{\varGamma}^{\mathsf{iso}}(n)$, $c_{\varGamma}^{\mathsf{rot}}(n)$ and $c_{\varGamma}(n)$ are supermultiplicative, that is, $c_{\varGamma}^{\mathsf{iso}}(mn) \geqslant c_{\varGamma}^{\mathsf{iso}}(m)\, c_{\varGamma}^{\mathsf{iso}}(n)$ holds for coprime integers m and n, and likewise for the other functions.* $\square$

Given the close relationship of similar sublattices and coincidence site lattices, which we will analyse below, one might be tempted to assume that the counting functions $b_{\varGamma}^{\mathsf{pr}}(n)$ and $b_{\varGamma}(n)$ for similar sublattices are multiplicative if and only if the corresponding counting functions $c_{\varGamma}(n)$ and $c_{\varGamma}^{\mathsf{iso}}(n)$ are multiplicative. However, this is not true. In fact, SSLs seem to be more prone to violation of multiplicativity than CSLs. For instance, for $\varGamma = \mathbb{Z} \times 5\mathbb{Z}$, multiplicativity is violated for $b_{\varGamma}^{\mathsf{pr}}(n)$ and $b_{\varGamma}(n)$, compare [17], while $c_{\varGamma}(n)$ and $c_{\varGamma}^{\mathsf{iso}}(n)$ are still multiplicative [36].

We expect that the connection between $c_{\varGamma}^{\mathsf{iso}}(n)$ and $c_{\varGamma}(n)$ must be closer, and in fact one has the following result.

Theorem 3.7.18 ([95, 97]). *If the arithmetic function $c_{\varGamma}^{\mathsf{iso}}(n)$ is multiplicative, then so is $c_{\varGamma}(n)$.* $\square$

It is presently unknown whether the converse holds or not. As the counting functions $c_{\varGamma}(n)$ and $c_{\varGamma}^{\mathsf{iso}}(n)$ are generally not multiplicative, it is desirable to have some criteria when they are. For $c_{\varGamma}(n)$, we have the following result.

Theorem 3.7.19 ([95, 97]). *For a lattice $\varGamma \subset \mathbb{R}^d$, the following statements are equivalent.*

(1) *The arithmetic function $c_{\varGamma}(m)$ is multiplicative.*

(2) *Every simple CSL $\varGamma(R)$ has a representation of the form*

$$\varGamma(R) \,=\, \varGamma(R_1) \cap \ldots \cap \varGamma(R_n)$$

with all indices $\varSigma_{\varGamma}(R_i)$ being powers of distinct primes.

(3) *Every MCSL $\varGamma(R_1, \ldots, R_n)$ of order n has a representation of the form $\varGamma(R_1, \ldots, R_n) = \varGamma_1 \cap \ldots \cap \varGamma_k$ where the $\varGamma_i$ are MCSLs of order at most n whose indices $\varSigma_i$ are powers of distinct primes.* $\square$

Let us mention that the representation $\varGamma(R) = \varGamma(R_1) \cap \ldots \cap \varGamma(R_n)$, if it exists, is unique up to the order of the $\varGamma(R_i)$. In fact, if $\Sigma(R) = p_1^{r_1} \cdots p_n^{r_n}$ is the prime factorisation of $\Sigma(R)$ and $m_i := \Sigma(R)\, p_i^{-r_i}$, then $\varGamma(R_i)$ can be calculated via

$$\varGamma(R_i) \,=\, \Big(\frac{1}{m_i}\varGamma(R)\Big) \cap \varGamma.$$

Note that the right-hand side is always a sublattice of $\varGamma$ of index $p_i^{r_i}$. The key in proving Theorem 3.7.19 is to show that it is actually a CSL if $c_{\varGamma}(m)$ is multiplicative. On the other hand, one can show that $\varGamma(R_1) \cap \ldots \cap \varGamma(R_n)$ is always a simple CSL if the indices are coprime, which allows one to count all CSLs that have such a representation. Analogous results hold for MCSLs; compare [95, 97].

A similar criterion exists for $c_{\varGamma}^{\mathsf{iso}}(n)$. In order to formulate it, we need some terminology. We call a bijection $\pi = \{p_1, p_2 \ldots\}$ from the positive integers onto the prime numbers an ordering of the prime numbers. We call a decomposition of a coincidence isometry $R = R_1 \cdots R_n$ a π-decomposition of R if, for any i, $\varSigma_{\varGamma}(R_i)$ is a power of p_i (we allow $\varSigma_{\varGamma}(R_i) = p_i^0 = 1$). It is clear that any π-decomposition is unique up to point group elements.

Theorem 3.7.20 ([95, 97])**.** *The following statements are equivalent.*

(1) *The arithmetic function $c_{\varGamma}^{\mathsf{iso}}(m)$ is multiplicative.*
(2) *There exists an ordering π of the prime numbers such that any coincidence isometry R has a (unique) π-decomposition.*
(3) *For any ordering π of the prime numbers, there exists a π-decomposition of every coincidence isometry R.* □

3.7.5. Generalisations to $\mathbb{Z}$-modules

The considerations on CSLs can be generalised to embedded $\mathbb{Z}$-modules. As most of the definitions and results depend only on the algebraic properties, their generalisation is straightforward. However, some of our previous proofs involved the use of the dual lattice, which has no immediate counterpart for $\mathbb{Z}$-modules. In these cases, some care and new approaches are needed.

We recall from Definition 3.6.3 that two embedded $\mathbb{Z}$-modules M_1 and M_2 are called commensurate, $M_1 \sim M_2$, if their intersection $M_1 \cap M_2$ has finite index in both M_1 and M_2. The notion of a coincidence site lattice can now easily be transferred to the case of modules as follows.

Definition 3.7.21. Let $M \subset \mathbb{R}^d$ be a properly embedded $\mathbb{Z}$-module of finite rank, and let $R \in \mathrm{O}(d, \mathbb{R})$. If $M \sim RM$, then $M(R) := M \cap RM$ is called a *coincidence site module* (CSM). In this case, R is called a *coincidence isometry*. The corresponding index $\varSigma_M(R) := [M : M(R)]$ is called its *coincidence index*.

Again, we are interested in the sets

$$\mathrm{OC}(M) := \{R \in \mathrm{O}(d,\mathbb{R}) \mid M \sim RM\} \tag{3.7.5}$$

and

$$\mathrm{SOC}(M) := \{R \in \mathrm{OC}(M) \mid \det(R) = 1\}. \tag{3.7.6}$$

As expected, these sets are indeed groups.

Theorem 3.7.22. *If $M \subset \mathbb{R}^d$ is a properly embedded $\mathbb{Z}$-module, the set of all coincidence isometries $\mathrm{OC}(M)$ forms a subgroup of $\mathrm{O}(d,\mathbb{R})$. Likewise, $\mathrm{SOC}(M)$ is a subgroup of $\mathrm{SO}(d,\mathbb{R})$.* □

Lemmas 3.7.2 and 3.7.3 immediately generalise as follows.

Lemma 3.7.23 ([97, Lemmas 3.1.2 and 3.1.3])**.** *The* OC*-groups are equal for commensurate modules.*

Moreover, similar modules have conjugate OC*-groups. In particular, one has $\mathrm{OC}(\alpha RM) = R\,\mathrm{OC}(M)\,R^{-1}$ and $\Sigma_{\alpha RM}(S) = \Sigma_M(R^{-1}SR)$.* □

Obviously, there is no analogue of Lemma 3.7.4. Thus, it is not evident whether an analogue of Lemma 3.7.5 exists. Fortunately, it does, but its proof requires some results on irreducible polynomials over the ring $\mathbb{Z}$; compare [97].

Theorem 3.7.24 ([97, Thm. 3.1.6])**.** *Let $M \subseteq \mathbb{R}^d$ be an embedded $\mathbb{Z}$-module of finite rank. For any $R \in \mathrm{OC}(M)$, we have $\Sigma_M(R) = \Sigma_M(R^{-1})$.* □

Again, it is interesting to compare the coincidence indices of modules with those of their submodules.

Theorem 3.7.25 ([97, Thm. 3.1.9])**.** *Let N be a submodule of M of index m. Then, $\Sigma_M(R)$ divides $m\Sigma_N(R)$ and $\Sigma_N(R)$ divides $m\Sigma_M(R)$.* □

Whereas the second statement of Lemma 3.7.9 can be generalised immediately, the first claim of Theorem 3.7.25 requires a different approach, as we generally lack the notion of a dual module. The proof is algebraic in nature and can be found in [97]; compare also [64], where a similar approach for lattices is described.

3.7.6. Similar versus coincidence submodules

After we have dealt with similar sublattices and coincidence site lattices and their generalisations, let us return to the connections between them. It is clear that there are substantial connections, as became obvious from the groups we defined along the way. In line with Section 3.3, let us illustrate this in more detail with the square lattice, the latter once again identified with $\mathbb{Z}[\mathrm{i}]$, the ring of Gaussian integers.

Example 3.7.26. We know from Theorem 3.5.14 and Example 3.5.15 that $\mathrm{SOS}(\mathbb{Z}[\mathrm{i}])$ is given by

$$\mathrm{SOS}(\mathbb{Z}[\mathrm{i}]) \,=\, \Big\{ \frac{z}{|z|} \;\Big|\; 0 \neq z \in \mathbb{Z}[\mathrm{i}] \Big\} \,\simeq\, C_8 \times \mathbb{Z}^{(\aleph_0)}.$$

In comparison, we have

$$\mathrm{SOC}(\mathbb{Z}[\mathrm{i}]) \,=\, \Big\{ \frac{z}{\bar{z}} \;\Big|\; 0 \neq z \in \mathbb{Z}[\mathrm{i}] \Big\} \,=\, \Big\{ \frac{z^2}{|z|^2} \;\Big|\; 0 \neq z \in \mathbb{Z}[\mathrm{i}] \Big\} \,\simeq\, C_4 \times \mathbb{Z}^{(\aleph_0)},$$

where C_4 is the groups of units of $\mathbb{Z}[\mathrm{i}]$, while a full set of generators of $\mathbb{Z}^{(\aleph_0)}$ is provided by $\{ \frac{\pi_p}{\overline{\pi_p}} = \frac{\pi_p^2}{|\pi_p|^2} \mid p \equiv 1 \bmod 4 \}$, where, for each p of this kind, π_p is one of the Gaussian primes with $\pi_p \overline{\pi_p} = p$. Comparing these with the set of generators for $\mathrm{SOS}(\mathbb{Z}[\mathrm{i}])$ in Example 3.5.15, one sees that all generators of $\mathrm{SOC}(\mathbb{Z}[\mathrm{i}])$ are squares of generators of $\mathrm{SOS}(\mathbb{Z}[\mathrm{i}])$, and we infer that

$$\mathrm{SOS}(\mathbb{Z}[\mathrm{i}]) / \mathrm{SOC}(\mathbb{Z}[\mathrm{i}]) \,\simeq\, C_2^{(\aleph_0)},$$

which means that the factor group $\mathrm{SOS}(\mathbb{Z}[\mathrm{i}]) / \mathrm{SOC}(\mathbb{Z}[\mathrm{i}])$ is an infinite Abelian 2-group; compare [42]. ♢

Let us now see how this observation can be put on a more general basis. We will formulate the main results immediately for modules; compare [96, 97]. For the special cases of lattices, we refer to [42]. The corresponding results for a special class of modules, namely the $\mathcal{S}$-lattices from Definition 3.6.2, can be found in [43].

Lemma 3.7.27 ([97, Lemma 3.2.1])**.** *Let $M \subseteq \mathbb{R}^d$ be a finitely generated free $\mathbb{Z}$-module. Then,*

(1) $R \in \mathrm{OC}(M)$ *if and only if* $1 \in \mathrm{scal}_M(R)$.
(2) $R \in \mathrm{O}(M)$ *if and only if* $1 \in \mathrm{Scal}_M(R)$. □

Here, $\mathrm{O}(M)$ is the point symmetry group of M. An immediate consequence for lattices is the following result.

Corollary 3.7.28. *If $\varGamma \subset \mathbb{R}^d$ is a lattice, one has $R \in \mathrm{OC}(\varGamma)$ if and only if $R \in \mathrm{OS}(\varGamma)$ together with $\mathrm{den}_{\varGamma}(R) \in \mathbb{N}$.* □

It is often helpful to know some connections between the coincidence indices and the corresponding denominators; compare [96].

Lemma 3.7.29. *Let $\varGamma$ be a lattice in $\mathbb{R}^d$. For any $R \in \mathrm{OC}(\varGamma)$, one has*

(1) $\mathrm{lcm}\big(\mathrm{den}_{\varGamma}(R), \mathrm{den}_{\varGamma}(R^{-1})\big)$ *divides* $\varSigma_{\varGamma}(R)$;
(2) $\varSigma_{\varGamma}(R)$ *divides* $\gcd\big(\mathrm{den}_{\varGamma}(R), \mathrm{den}_{\varGamma}(R^{-1})\big)^d$.
(3) $\varSigma_{\varGamma}(R)^2$ *divides* $\mathrm{lcm}\big(\mathrm{den}_{\varGamma}(R), \mathrm{den}_{\varGamma}(R^{-1})\big)^d$.

PROOF. For (1), recall that $\Gamma(R)$ has index $\Sigma(R)$ in Γ, thus

$$\Sigma(R)\Gamma \subseteq \Gamma(R) \subseteq R\Gamma,$$

or, equivalently, $\Sigma(R)R^{-1}\Gamma \subseteq \Gamma$. Consequently, $\Sigma(R)$ is a multiple of $\mathrm{den}(R^{-1})$. By symmetry, $\mathrm{den}(R)$ is a divisor of $\Sigma(R^{-1}) = \Sigma(R)$ as well, and claim (1) follows.

For (2), we exploit that $\mathrm{den}(R)$ is an integer for $R \in \mathrm{OC}(\Gamma)$. Consequently, $\mathrm{den}(R)R\Gamma$ is a sublattice of both Γ and $R\Gamma$, wherefore one has $\mathrm{den}(R)R\Gamma \subseteq \Gamma(R)$. Comparing the indices of $\mathrm{den}(R)R\Gamma$ and $\Gamma(R)$ in Γ shows that $\Sigma(R)$ divides $\mathrm{den}(R)^d$. Using $\Sigma(R^{-1}) = \Sigma(R)$ as above yields (2).

Finally, let $a := \mathrm{lcm}\big(\mathrm{den}(R), \mathrm{den}(R^{-1})\big)$. Then, $a\Gamma$ and $aR\Gamma$ are both sublattices of Γ and of $R\Gamma$, hence $a(\Gamma + R\Gamma)$ is a sublattice of $\Gamma \cap R\Gamma$ with index

$$[R\cap R\Gamma : a(\Gamma + R\Gamma)] \;=\; \frac{a^d}{\Sigma(R)^2},$$

as $\Sigma(R) = [\Gamma : \Gamma(R)] = [\Gamma + R\Gamma : \Gamma]$. Hence $\Sigma(R)^2$ divides a^d. □

The situation becomes particularly simple for planar lattices, where we get the following result by recalling $\mathrm{den}_\Gamma(R) = \mathrm{den}_\Gamma(R^{-1})$.

Corollary 3.7.30 ([96, Cor. 2.6])**.** *Let Γ be a lattice in $\mathbb{R}^2$. Then, for any $R \in \mathrm{OC}(\Gamma)$, one has $\Sigma_\Gamma(R) = \mathrm{den}_\Gamma(R)$.* □

Our main result follows from Theorem 3.6.12.

Theorem 3.7.31 ([97, Thm. 3.2.2])**.** *Let $M \subset \mathbb{R}^d$ be an embedded $\mathbb{Z}$-module of finite rank. Then, the kernel of the homomorphism*

$$\begin{aligned}\phi\colon \mathrm{OS}(M) &\longrightarrow \mathbb{R}_+/(\mathrm{scal}_M(\mathbb{1}) \cap \mathbb{R}_+),\\ R &\longmapsto \mathrm{scal}_M(R) \cap \mathbb{R}_+,\end{aligned}$$

is the group $\mathrm{OC}(M)$. Thus, $\mathrm{OC}(M)$ is a normal subgroup of $\mathrm{OS}(M)$, and $\mathrm{OS}(M)/\mathrm{OC}(M)$ is Abelian. □

This result was first proved for lattices in [42] and later generalised to $\mathcal{S}$-lattices in [43].

If $M \subseteq \mathbb{R}^d$ is a lattice or an $\mathcal{S}$-lattice, all elements of $\mathrm{OS}(M)/\mathrm{OC}(M)$ have finite order. In particular, their order is a divisor of d; see [42, 43].

Theorem 3.7.32. *Let $M \subseteq \mathbb{R}^d$ be a lattice or an $\mathcal{S}$-lattice. Then, the factor group $\mathrm{OS}(M)/\mathrm{OC}(M)$ is the direct sum of cyclic groups of prime power order that divide d.* □

The close relationship between SSLs and CSLs is also reflected in the following condition for two CSLs to be equal.

Lemma 3.7.33 ([97, Lemma 3.4.2]). *Let $\varGamma \subset \mathbb{R}^d$ be a lattice. Assume that $R_1, R_2 \in \mathrm{OC}(\varGamma)$ generate the same CSL, so $\varGamma(R_1) = \varGamma(R_2)$. Then, one has $\varSigma(R_1) = \varSigma(R_2)$ and $\mathrm{den}(R_1^{-1}) = \mathrm{den}(R_2^{-1})$.*

Proof. The statement about $\varSigma$ is trivial. For the denominator, observe that

$$\mathrm{den}(R_1^{-1})\varGamma \subseteq \varGamma(R_1) = \varGamma(R_2) \subseteq R_2\varGamma.$$

Consequently,

$$\mathrm{den}(R_1^{-1})R_2^{-1}\varGamma \subseteq \varGamma,$$

which shows that $\mathrm{den}(R_1^{-1})$ is a multiple of $\mathrm{den}(R_2^{-1})$. Then, by symmetry, $\mathrm{den}(R_2^{-1})$ is a multiple of $\mathrm{den}(R_1^{-1})$ as well, and the claim follows. □

This result is particularly useful in the following examples, when we have to characterise those coincidence isometries that generate the same CSL. Let us start our series of illustrations with some examples in the plane.

3.8. (M)CSMs of planar modules with N-fold symmetry

We can generalise the results of the square lattice to all rings $\mathbb{Z}[\xi_n]$ of cyclotomic integers which are PIDs; compare [71, 8]. Thus, let n be one of the numbers given in Eq. (3.5.11). We have seen in Section 3.5.2 that the similar submodules are then exactly the non-trivial ideals of $\mathbb{Z}[\xi_n]$, and that the similarity rotations are given by $\frac{v}{|v|}$ with $v \in \mathbb{Z}[\xi_n]$.

As any of these 29 modules is also a ring, we have $\mathrm{MR}(\mathbb{Z}[\xi_n]) = \mathbb{Z}[\xi_n]$. This implies that the coincidence rotations are precisely given by $\mathrm{e}^{\mathrm{i}\varphi} = \frac{v}{|v|}$ for which $|v|^2 = v\bar{v}$ is a square in $\mathbb{Z}[\xi_n]$. In other words, using the unique prime factorisation up to units in $\mathbb{Z}[\xi_n]$, the coincidence rotations are precisely the rotations of the form $\varepsilon\frac{w}{\overline{w}}$ with $0 \neq w \in \mathbb{Z}[\xi_n]$, where ε is a unit in $\mathbb{Z}[\xi_n]$. Here, we may assume that $\frac{w}{\overline{w}}$ is a reduced fraction, which means that w and $\overline{w}$ are coprime. Under this assumption, one finds

$$\mathbb{Z}[\xi_n] \cap \varepsilon\frac{w}{\overline{w}}\mathbb{Z}[\xi_n] = w\mathbb{Z}[\xi_n]. \tag{3.8.1}$$

To find the possible values of w, we mention that a prime $\omega \in \mathbb{Z}[\xi_n]$ can be a factor of w only if $\frac{\omega}{\bar{\omega}}$ is not a unit in $\mathbb{Z}[\xi_n]$. Thus, we only have to consider the so-called *complex splitting primes*. To expand on this, consider the prime factorisation of a rational prime p over the real subring $\mathcal{O}_n = \mathbb{Z}[\xi_n + \bar{\xi}_n]$, which is the ring of integers of the maximal real subfield $\mathbb{Q}(\xi_n + \bar{\xi}_n)$ of $\mathbb{Q}(\xi_n)$. Let π be a prime in $\mathcal{O}_n$. Now, the complex splitting primes are those primes π that split as $\pi = \omega_\pi\bar{\omega}_\pi$ over $\mathbb{Z}[\xi_n]$, with ω_π and $\bar{\omega}_\pi$ being non-associated primes in $\mathbb{Z}[\xi_n]$, which means that $\frac{\omega_\pi}{\bar{\omega}_\pi}$ is not a unit. Thus, the possible values of w are of the form

$$w = \varepsilon\prod_{\pi}\omega_\pi^{t_\pi^+}\bar{\omega}_\pi^{t_\pi^-}, \tag{3.8.2}$$

where ε is a unit, $t_\pi^+ t_\pi^- = 0$, and the product runs over all primes $\pi \in \mathcal{O}_n$ that divide $w\overline{w}$. In other words, any coincidence rotation in $\mathrm{SOC}(\mathbb{Z}[\xi_n])$ can be written as a finite product

$$\mathrm{e}^{\mathrm{i}\varphi} \,=\, \varepsilon' \frac{w}{\overline{w}} \,=\, \varepsilon' \prod_\pi \left(\frac{\omega_\pi}{\overline{\omega}_\pi} \right)^{t_\pi}, \tag{3.8.3}$$

with $t_\pi = t_\pi^+ - t_\pi^-$, where π runs over the complex splitting primes of $\mathcal{O}_n$ and where ε' is again a unit.

Any complex splitting prime $\pi \in \mathcal{O}_n$ lies over a unique rational prime p, which is the norm of π in $\mathcal{O}_n$. Then, one also calls p a complex splitting prime of the field extension $\mathbb{Q}(\xi_n)/\mathbb{Q}$. The set of all such rational primes is abbreviated as $\mathcal{C}_n$ and thus consists of all rational primes that split in the final step from $\mathbb{Q}(\xi_n + \bar{\xi}_n)$ to $\mathbb{Q}(\xi_n)$. To expand on the structure of the primes and their splitting, we recall that the index $\big[\mathbb{Z}[\xi_n] : \omega_\pi \mathbb{Z}[\xi_n]\big] = p^{\ell_p}$ depends only on p, where ℓ_p is an integer which we will specify below. As a result, the CSM $\mathbb{Z}[\xi_n] \cap \varepsilon \frac{w}{\overline{w}} \mathbb{Z}[\xi_n] = w\mathbb{Z}[\xi_n]$ has index

$$\Sigma_{\mathbb{Z}[\xi_n]}\big(\varepsilon \tfrac{w}{\overline{w}}\big) \,= \prod_\pi p^{\ell_p |t_\pi|} \tag{3.8.4}$$

with t_π as introduced above. Thus, the possible coincidence indices are products of the so-called *basic indices* p^{ℓ_p}, and the coincidence spectrum is the (multiplicative) monoid generated by these basic indices. In other words,

$$\sigma\big(\mathbb{Z}[\xi_n]\big) \,=\, \Big\{ \prod_{p \in \mathcal{C}_n} p^{\ell_p t_p} \,\Big|\, t_p \in \mathbb{N}, \text{only finitely many } t_p \neq 0 \Big\}, \tag{3.8.5}$$

where $\mathcal{C}_n$ is the set of complex splitting primes as introduced above.

As $\mathbb{Z}[\xi_n]$ is a PID for the list of n we consider here, the counting function $c_n(m) = c_{\mathbb{Z}[\xi_n]}(m)$ is multiplicative, wherefore it suffices to determine it for $m = p^{\ell_p}$. This is now a purely combinatorial task, and one finally arrives at the following result.

Theorem 3.8.1 ([71, Thm. 3] and [8, Thm. 1])**.** *Let n be one of the* 29 *numbers from Eq.* (3.5.11)*. Then, the generating function for the number $c_n(m) = c_{\mathbb{Z}[\xi_n]}(k)$ of CSMs of $\mathbb{Z}[\xi_n]$ of index k is given by*

$$\Psi_{\mathbb{Z}[\xi_n]}(s) \,=\, \sum_{k=1}^{\infty} \frac{c_n(k)}{k^s} \,=\, \frac{\zeta_{\mathbb{K}_n}(s)}{\zeta_{\mathbb{L}_n}(2s)} \begin{cases} (1+p^{-s})^{-1}, & \text{if } n = p^r, \\ 1, & \text{otherwise,} \end{cases}$$

where $\zeta_{\mathbb{K}_n}(s)$ and $\zeta_{\mathbb{L}_n}(2s)$ are the Dedekind zeta functions of the number field $\mathbb{K}_n = \mathbb{Q}(\xi_n)$ and its maximal real subfield $\mathbb{L}_n = \mathbb{Q}(\xi_n + \bar{\xi}_n)$, respectively. If $\mathcal{C}_n$ denotes the set of complex splitting primes for the field extension $\mathbb{K}_n/\mathbb{Q}$,

then $\Psi_{\mathbb{Z}[\xi_n]}(s)$ *has the Euler product expansion*

$$\Psi_{\mathbb{Z}[\xi_n]}(s) \,=\, \prod_{p\in\mathcal{C}_n} \left(\frac{1+p^{-\ell_p s}}{1-p^{-\ell_p s}}\right)^{\frac{m_p}{2}} ,$$

with certain integers ℓ_p *and* m_p *as follows. If* $p\nmid n$*, one has* $m_p = \frac{\phi(n)}{\ell_p}$ *where* ℓ_p *is the smallest positive integer such that* $p^{\ell_p} \equiv 1 \bmod n$*. If* $p|n$ *together with* $n = p^t r$*, where* r *and* p *are coprime, one has* $m_p = \frac{\phi(r)}{\ell_p}$ *where* ℓ_p *is the smallest positive integer such that* $p^{\ell_p} \equiv 1 \bmod r$*.* □

For explicit values of ℓ_p and m_p, see [8, Tables 1 and 2]. The first terms of $\Psi_{\mathbb{Z}[\xi_n]}(s)$ for all n from Eq. (3.5.11) are listed in [8, Table 4].

The explicit expression of $\Psi_{\mathbb{Z}[\xi_n]}(s)$ in terms of zeta functions allows us to determine the asymptotic behaviour of $c_n(k)$. Here, $\Psi_{\mathbb{Z}[\xi_n]}(s)$ is a meromorphic function that is analytic in the half-plane $\{\mathrm{Re}(s) > 1\}$ and has a simple pole at $s = 1$, which results in linear growth for the summatory function of $c_n(k)$. In particular, using Theorem 3.4.1, we get the following result.

Corollary 3.8.2 ([8, Cor. 1])**.** *The asymptotic behaviour of the number* $c_n(k)$ *of CSMs of* $\mathbb{Z}[\xi_n]$ *of index* k *is given by*

$$\sum_{k\leqslant x} c_n(k) \;\sim\; \gamma_n\, x$$

as $x\to\infty$*, where* γ_n *is the residue of* $\Psi_{\mathbb{Z}[\xi_n]}(s)$ *at* $s = 1$*, which is given by*

$$\gamma_n \;=\; \frac{\alpha_n}{\zeta_{\mathbb{L}_n}(2)} \begin{cases} p/(p+1), & \text{if } n = p^r, \\ 1, & \text{otherwise,} \end{cases}$$

with $\alpha_n := \mathrm{res}_{s=1}\big(\zeta_{\mathbb{K}_n}(s)\big)$*.* □

Note that the constants α_n and γ_n can be calculated by expressing $\zeta_{\mathbb{K}_n}(s)$ and $\zeta_{\mathbb{L}_n}(s)$ in terms of Riemann's zeta function $\zeta(s)$ and certain L-series; compare [8, Sec. 4]. For some examples including $n \in \{3,4,5,7,8,12\}$, we refer to [71, Sec. 4], where the average $\gamma_n = \lim_{x\to\infty} \frac{1}{x}\sum_{k\leqslant x} c_n(k)$ has been evaluated explicitly. Numerical values for α_n and γ_n are listed in [8, Table 3].

Let us continue with multiple coincidences. As any MCSM is an intersection of simple CSMs, we see that

$$\begin{aligned} &\mathbb{Z}[\xi_n] \cap \varepsilon_1 \frac{w_1}{\overline{w}_1}\mathbb{Z}[\xi_n] \cap \ldots \cap \varepsilon_k \frac{w_k}{\overline{w}_k}\mathbb{Z}[\xi_n] \\ &\qquad = \; w_1\mathbb{Z}[\xi_n] \cap \ldots \cap w_k\mathbb{Z}[\xi_n] \;=\; w\mathbb{Z}[\xi_n] \end{aligned} \tag{3.8.6}$$

with $w = \operatorname{lcm}(w_1, \ldots, w_k)$. Again, any MCSM is an ideal of $\mathbb{Z}[\xi_n]$, but w is more general now. Nevertheless, w is still of the form of a finite product,

$$w \,=\, \varepsilon \prod_{\pi} \omega_{\pi}^{t_{\pi}^{+}} \bar{\omega}_{\pi}^{t_{\pi}^{-}}, \tag{3.8.7}$$

but now without any further restriction on the non-negative integers t_{π}^{+} and t_{π}^{-}. This shows that the coincidence spectrum does not change, so that

$$\sigma\big(\mathbb{Z}[\xi_n]\big) \,=\, \sigma_{\infty}\big(\mathbb{Z}[\xi_n]\big); \tag{3.8.8}$$

compare [8, Cor. 2].

It follows from Eq. (3.8.6) that any MCSM can actually be written as the intersection of only two simple CSMs. This allows one to determine the number $c_n^{\infty}(k)$ of MCSMs of $\mathbb{Z}[\xi_n]$ of index k. The result reads as follows.

Theorem 3.8.3 ([71, Thm. 3] and [8, Thm. 1])**.** *Let n be one of the* 29 *numbers from Eq.* (3.5.11)*. Then, the generating function for the number $c_n^{\infty}(k) = c_{\mathbb{Z}[\xi_n]}^{\infty}(k)$ of CSMs of $\mathbb{Z}[\xi_n]$ of index k is given by*

$$\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s) \,=\sum_{k=1}^{\infty} \frac{c_n^{\infty}(k)}{k^s} \,=\, \prod_{p \in \mathcal{C}_n} \Big(\frac{1}{1-p^{-\ell_p s}}\Big)^{m_p},$$

where $\mathcal{C}_n$ denotes the set of complex splitting primes for the field extension $\mathbb{K}_n/\mathbb{Q}$ and the integers ℓ_p and m_p are those from Theorem 3.8.1*.* □

This nice generating function is due to the fact that we actually count all ideals whose index m factors into primes contained in $\mathcal{C}_n$. As $\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s)$ still has a simple pole at $s = 1$, using Theorem 3.4.1 once more, we get a linear growth behaviour again. The determination of the residue is a bit more complicated here, as $\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s)$ cannot be represented via zeta functions in a simple way. Still, one has the following result.

Corollary 3.8.4 ([8, Cor. 1])**.** *The summatory function $\sum_{k \leqslant x} c_n^{\infty}(k)$ has the asymptotic behaviour*

$$\sum_{k \leqslant x} c_n^{\infty}(k) \,\sim\, \beta_n \, x$$

as $x \to \infty$, with the growth constant $\beta_n = \operatorname{res}_{s=1}\big(\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s)\big) = q_n \gamma_n$. Here, γ_n is defined as in Corollary 3.8.2*, and q_n is given by*

$$q_n \,:=\, \lim_{s \to 1} \frac{\Psi_{\mathbb{Z}[\xi_n]}^{\infty}(s)}{\Psi_{\mathbb{Z}[\xi_n]}(s)} \,=\prod_{\ell=1}^{\infty} \big(\Psi_{\mathbb{Z}[\xi_n]}(2^{\ell})\big)^{2^{-\ell}}. \qquad \square$$

The last formula in Corollary 3.8.4 is a consequence of the representation

$$\begin{aligned}\Psi^{\infty}_{\mathbb{Z}[\xi_n]}(s) \;&=\; \bigl(\Psi^{\infty}_{\mathbb{Z}[\xi_n]}(2^{L+1}s)\bigr)^{2^{-(L+1)}} \prod_{\ell=0}^{L} \bigl(\Psi_{\mathbb{Z}[\xi_n]}(2^{\ell}s)\bigr)^{2^{-\ell}} \\ &=\; \Psi_{\mathbb{Z}[\xi_n]}(s) \prod_{\ell=1}^{\infty} \bigl(\Psi_{\mathbb{Z}[\xi_n]}(2^{\ell}s)\bigr)^{2^{-\ell}},\end{aligned} \tag{3.8.9}$$

which holds for any integer $L \geqslant 0$; compare [8, Prop. 2]. As the infinite product converges rapidly, q_n, and thus β_n, can be calculated numerically in an efficient way; see [8, Table 3] for a list of values of β_n.

Example 3.8.5. Let us once more consider the square lattice for illustration. Theorem 3.8.3 implies that the generating function for its MCSLs reads

$$\begin{aligned}\Psi^{\infty}_{\square}(s) \;&=\; \sum_{m=1}^{\infty} \frac{c^{\infty}_{\square}(k)}{k^s} \;=\; \bigl(1+2^{-s}\bigr)^{-1} \frac{\zeta_K(s)}{\zeta(2s)} \\ &=\; \prod_{p\equiv 1\,(4)} \frac{1}{(1-p^{-s})^2} \;=\; \Psi_{\square}(s) \prod_{p\equiv 1\,(4)} \frac{1}{1-p^{-2s}},\end{aligned}$$

where we have employed the notation $c^{\infty}_{\square}(k) = c^{\infty}_{4}(k)$ for the number of MCSLs. The latter is a multiplicative function, whose values for (positive) prime powers are given by

$$c^{\infty}_{\square}(p^r) = \begin{cases} r+1, & \text{if } p \equiv 1 \bmod 4, \\ 0, & \text{otherwise.} \end{cases}$$

The first terms of the expansion read

$$\Psi^{\infty}_{\square}(s) \;= 1 + \frac{2}{5^s} + \frac{2}{13^s} + \frac{2}{17^s} + \frac{3}{25^s} + \frac{2}{29^s} + \frac{2}{37^s} + \frac{2}{41^s} + \frac{2}{53^s} + \ldots,$$

and a comparison with $\Psi_{\square}(s)$ from Eq. (3.3.5) yields

$$\Psi^{\infty}_{\square}(s) - \Psi_{\square}(s) \;=\; \frac{1}{25^s} + \frac{2}{125^s} + \frac{1}{169^s} + \frac{1}{289^s} + \frac{2}{325^s} + \frac{2}{425^s} + \frac{3}{625^s} + \ldots;$$

compare [8, Table 5]. Note that no additional MCSLs exist for square-free indices. The first terms of $\Psi^{\infty}_{\square}(s) - \Psi_{\square}(s)$ indicate that most MCSLs actually are simple CSLs, which is confirmed by the asymptotic growth rates of the summatory functions,

$$\gamma_{\square} := \gamma_4 = \frac{1}{\pi} \approx 0.318310 \quad \text{and} \quad \beta_{\square} := \beta_4 \approx 0.336193,$$

of the simple and multiple CSLs, respectively; compare [8, Table 3].

Furthermore, note that the simple CSLs are all primitive SSLs, whereas the additional MCSLs are all non-primitive SSLs. In fact, an SSL is an MCSL if and only if its index factors into primes $p \equiv 1 \bmod 4$ only.

The possible coincidence indices are precisely the positive odd integers that are products of primes $p \equiv 1 \bmod 4$ only. In other words, the coincidence spectra of the square lattice are given by

$$\sigma(\mathbb{Z}^2) \,=\, \sigma_{\infty}(\mathbb{Z}^2) \,=\, \{\text{all finite products of primes} \equiv 1 \bmod 4\}$$

and thus agree in this case. ◊

Let us now turn our attention to some important examples in three and four dimensions, where quaternions will play a fundamental role; compare Section 3.4.1. On the one hand, following Cayley, rotations in three and four dimensions can be parametrised conveniently by quaternions, which allows us to exploit the algebraic structure of certain rings of quaternions, including the rings $\mathbb{J}$, $\mathbb{L}$ and $\mathbb{I}$. On the other hand, these rings are either four-dimensional lattices themselves, like $\mathbb{J}$ and $\mathbb{L}$, or they are related to lattices. For instance, the lattice A_4 is related to the icosian ring $\mathbb{I}$; see Section 3.11.1. Likewise, the projections of $\mathbb{J}$ and $\mathbb{L}$ onto the three-dimensional imaginary subspace yield the body-centred and primitive cubic lattices, respectively. Moreover, $\mathbb{I}$ is a $\mathbb{Z}[\tau]$-lattice of rank 4 in the sense of Definition 3.6.2.

3.9. The cubic lattices

The three-dimensional cubic lattices are among the most important lattices in crystallography, and the study of their coincidences is a classic problem [74, 46, 48, 47]. Later, these lattices have been revisited in a more mathematical context [4, 92]. Here, the key tool is the ring $\mathbb{J}$ of Hurwitz quaternions, since it turns out that any coincidence rotation of a three-dimensional cubic lattice can be parametrised by a Hurwitz quaternion; compare [AO1, Sec. 2.5.4] as well as [11] and references therein for some general background.

Let us first define our setting. We use the conventions of [AO1, Ex. 3.2] and define

$$\varGamma_{\mathsf{pc}} \,:=\, \mathbb{Z}^3, \quad \varGamma_{\mathsf{bcc}} \,:=\, \mathbb{Z}^3 \cup (u + \mathbb{Z}^3), \quad \varGamma_{\mathsf{fcc}} \,:=\, \varGamma_{\mathsf{bcc}}^{*}, \tag{3.9.1}$$

with $u = \frac{1}{2}(1,1,1)$. Here, the index pc indicates that this lattice is a primitive cubic lattice, and likewise bcc and fcc denote the body-centred and the face-centred cubic lattices, respectively.

Traditionally, one starts with the primitive cubic lattice, partly due to the fact that this lattice allows the easiest treatment with elementary methods. We will deviate from this tradition here, as the body-centred lattice allows for the nicest description of its coincidence site lattices.

Fact 3.9.1. *One has* $\varGamma_{\mathsf{bcc}} \simeq \mathrm{Im}(\mathbb{J})$ *and* $\varGamma_{\mathsf{pc}} \simeq \mathrm{Im}(\mathbb{L})$. □

Recall that $\mathbb{J}$ is a maximal order and a principal ideal ring, whereas $\mathbb{L}$ is neither. This indicates that Γ_{bcc} is easier to deal with, because we can exploit the arithmetic properties of $\mathbb{J}$ while relying on its ideal structure.

The first step in determining the CSLs of Γ is the determination of $\mathrm{OC}(\Gamma)$. Since the point reflection $I\colon x \mapsto -x$ is a symmetry operation of all three-dimensional lattices, it is actually sufficient to determine $\mathrm{SOC}(\Gamma)$. We get the following well-known result; compare [4, 12, 97].

Theorem 3.9.2. *Let $\Gamma_{\mathsf{pc}}, \Gamma_{\mathsf{bcc}}, \Gamma_{\mathsf{fcc}} \subset \mathbb{R}^3$ be the primitive, the body-centred, and the face-centred cubic lattice of Eq.* (3.9.1)*, respectively. Then, one has $\mathrm{OC}(\Gamma_{\mathsf{pc}}) = \mathrm{OC}(\Gamma_{\mathsf{bcc}}) = \mathrm{OC}(\Gamma_{\mathsf{fcc}}) = \mathrm{O}(3,\mathbb{Q})$ together with*

$$\Sigma_{\mathsf{pc}}(R) \,=\, \Sigma_{\mathsf{bcc}}(R) \,=\, \Sigma_{\mathsf{fcc}}(R)$$

for all $R \in \mathrm{O}(3,\mathbb{Q})$.

Proof. The equality of the three OC-groups is a consequence of the fact that the three cubic lattices are mutually commensurate. The explicit form of the OC-group is most easily seen for the lattice $\Gamma_{\mathsf{pc}} = \mathbb{Z}^3$, since the standard basis of $\mathbb{R}^3$ is also a lattice basis of $\mathbb{Z}^3$.

Note that $\Gamma_{\mathsf{pc}} \subset \Gamma_{\mathsf{bcc}}$ is a sublattice of index 2. One easily verifies that $|x|^2$ is an integer for all $x \in \Gamma_{\mathsf{pc}}$ and that $4|x|^2 \equiv 3 \bmod 4$ for all $x \in \Gamma_{\mathsf{bcc}} \setminus \Gamma_{\mathsf{pc}}$. Hence, an application of Lemma 3.7.10 shows that $\Sigma_{\mathsf{pc}}(R)$ divides $\Sigma_{\mathsf{bcc}}(R)$. The reverse divisibility property can be obtained by considering the dual lattice $\Gamma^*_{\mathsf{bcc}} = \Gamma_{\mathsf{fcc}}$. In particular, $|x|^2$ is even for all $x \in \Gamma^*_{\mathsf{bcc}}$ and odd for all $x \in \Gamma_{\mathsf{pc}} \setminus \Gamma^*_{\mathsf{bcc}}$. □

Note that this result was already proved by Grimmer, Bollmann and Warrington [48]. Actually, they used a similar method in their proof, and Lemma 3.7.10 is a natural generalisation of their approach.

Remark 3.9.3. Let us note that $\mathrm{OC}(\Gamma) = \mathrm{OS}(\Gamma) = \mathrm{O}(3,\mathbb{Q})$ holds for all cubic lattices of Eq. (3.9.1). We have determined $\mathrm{OC}(\Gamma)$ explicitly above, but we could have argued more abstractly by using the connection of $\mathrm{OS}(\Gamma)$ and $\mathrm{OC}(\Gamma)$ as laid out in Section 3.7.6. It follows from Theorem 3.7.32 that all elements of $\mathrm{OS}(\Gamma)/\mathrm{OC}(\Gamma)$ have an order that divides 3. On the other hand, the cubic lattices are rational lattices, which implies that all elements of $\mathrm{OS}(\Gamma)/\mathrm{OC}(\Gamma)$ have an order at most 2. Thus, we indeed have $\mathrm{OC}(\Gamma) = \mathrm{OS}(\Gamma)$. Moreover, as Γ is commensurate to $\mathbb{Z}^3$, the elements of $\mathrm{OC}(\Gamma)$ are exactly the rational orthogonal matrices, $\mathrm{O}(3,\mathbb{Q})$. ◊

As any rotation in $\mathrm{O}(3,\mathbb{Q})$ can be parametrised by a rational quaternion, we can parametrise the coincidence rotations by primitive Lipschitz or Hurwitz quaternions. Contrary to the traditional approach in crystallography, we opt for primitive Hurwitz quaternions here; compare [4]. In particular,

via Eq. (3.4.1), one finds

$$\mathrm{SOC}(\Gamma_{\mathsf{bcc}}) = \{R(q) \mid q \in \mathbb{J}\} = \{R(q) \mid q \in \mathbb{J} \text{ is primitive}\}. \tag{3.9.2}$$

The first step in determining the coincidence index is the calculation of the denominator $\mathrm{den}_\Gamma(R(q))$. From Eq. (3.4.1), we see that $\mathrm{den}_\Gamma(R(q))$ must be a divisor of $|q|^2$. Taking into account that the greatest common divisor of all matrix entries of $R(q)$ is a power of 2, we get the following result.

Corollary 3.9.4. *For any cubic lattice Γ in the setting of Eq.* (3.9.1)*, we have* $\mathrm{den}_\Gamma(R(q)) = \frac{|q|^2}{2^\ell}$*, where q is a primitive Hurwitz quaternion and ℓ is the maximal exponent such that $2^\ell \big| |q|^2$.* □

Note that ℓ is either 0 or 1, depending on whether $|q|^2$ is odd or even. If one chooses to use primitive Lipschitz quaternions, one gets $\ell \in \{0, 1, 2\}$ instead. Furthermore, note that the denominators for any similarity rotation R and its inverse are the same, $\mathrm{den}_\Gamma(R^{-1}) = \mathrm{den}_\Gamma(R)$, as $R^{-1}(q) = R(\bar{q})$.

Proposition 3.9.5. *For any cubic lattice $\Gamma \subset \mathbb{R}^3$ as in Eq.* (3.9.1)*, we have*

$$\Sigma_\Gamma(R(q)) = \mathrm{den}_\Gamma(R(q)) = \frac{|q|^2}{2^\ell},$$

where q is a primitive Hurwitz quaternion and ℓ is the maximal exponent such that $2^\ell \big| |q|^2$.

Proof. From Theorem 3.7.29, we know that the index $\Sigma_\Gamma(R(q))$ is a multiple of $\mathrm{den}_\Gamma(R(q)) = \frac{|q|^2}{2^\ell}$ and a divisor of $\mathrm{den}_\Gamma(R(q))^2$. As the latter is odd, so is $\Sigma_\Gamma(R(q))$, and it is thus sufficient to show that $\Sigma_\Gamma(R(q))$ divides $|q|^2$.

By Theorem 3.9.2, the coincidence indices are the same for all cubic lattices. Hence, it suffices to prove that $\Sigma_{\mathsf{bcc}}(R(q))$ divides $|q|^2$. We observe $R(q)\,\mathrm{Im}(xq) = \mathrm{Im}(qx)$, which implies that $R(q)\,\mathrm{Im}(\mathbb{J}q) = \mathrm{Im}(q\mathbb{J})$, from which we infer that $\mathrm{Im}(q\mathbb{J}) \subseteq \Gamma_{\mathsf{bcc}}(R(q))$. Consequently, $\Sigma_{\mathsf{bcc}}(R(q))$ divides the index $[\mathrm{Im}(\mathbb{J}) : \mathrm{Im}(q\mathbb{J})]$.

In order to determine the latter, we note that $[\mathbb{J} : q\mathbb{J}] = |q|^4$ for any $q \in \mathbb{J}$. Moreover, one has

$$\big[\big(\mathbb{J} \cap \mathrm{Re}(\mathbb{H})\big) : \big((q\mathbb{J}) \cap \mathrm{Re}(\mathbb{H})\big)\big] = |q|^2,$$

where $\mathrm{Re}(\mathbb{H})$ is to be understood as the real axis. Hence $[\mathrm{Im}(\mathbb{J}) : \mathrm{Im}(q\mathbb{J})] = \frac{[\mathbb{J}:q\mathbb{J}]}{[\mathrm{Re}(\mathbb{J}):\mathrm{Re}(q\mathbb{J})]} = |q|^2$, and $\Sigma_{\mathsf{bcc}}(R(q))$ thus divides $|q|^2$. □

If $\mathrm{den}_\Gamma(R(q))$ is square-free, there exists a simple alternative proof. As $\mathrm{den}_\Gamma(R) = \mathrm{den}_\Gamma(R^{-1})$ for the cubic lattices, Theorem 3.7.29 tells us that $\Sigma_\Gamma(R)^2$ divides $\mathrm{den}_\Gamma(R)^3$, and if $\mathrm{den}_\Gamma(R)$ is square-free, we may infer that $\Sigma_\Gamma(R) = \mathrm{den}_\Gamma(R)$.

Remark 3.9.6. It follows from Proposition 3.9.5 that the coincidence indices are odd positive integers. Moreover, Lagrange's four-square theorem [51] tells us that any positive integer is a sum of four squares. Hence, for any odd n, there exists a Hurwitz quaternion q such that $n = |q|^2$. This implies that any odd positive integer is realised as a coincidence index, or in other words, the coincidence spectrum of any cubic lattice is precisely the set of positive odd integers, so $\sigma(\Gamma_{\mathsf{bcc}}) = \sigma(\Gamma_{\mathsf{pc}}) = \sigma(\Gamma_{\mathsf{fcc}}) = 2\mathbb{N}_0 + 1$. ◊

Proposition 3.9.7. *If q is a primitive Hurwitz quaternion with $|q|^2$ odd, one has $\Gamma_{\mathsf{bcc}}(R(q)) = \mathrm{Im}(q\mathbb{J})$.*

Proof. We have seen $\mathrm{Im}(q\mathbb{J}) \subseteq \Gamma_{\mathsf{bcc}}(R(q))$ in the proof of Proposition 3.9.5. If $|q|^2$ is odd, then both sublattices have the same index,

$$\Sigma_{\mathsf{bcc}}(R(q)) \,=\, |q|^2 \,=\, [\mathrm{Im}(\mathbb{J}) : \mathrm{Im}(q\mathbb{J})],$$

and hence $\mathrm{Im}(q\mathbb{J}) = \Gamma_{\mathsf{bcc}}(R(q))$. □

If $|q|^2$ is even, q can be written as $q = rs$ with $r, s \in \mathbb{J}$, where $|r|^2$ is odd and $|s|^2 = 2^\ell$. As $R(s)$ is a symmetry operation of Γ_{bcc}, we see that $\Gamma_{\mathsf{bcc}}(R(q)) = \Gamma_{\mathsf{bcc}}(R(r)) = \mathrm{Im}(r\mathbb{J})$.

An analogous result exists for the primitive cubic lattice $\mathbb{Z}^3$ and can be stated as follows; compare [97, Thm. 3.5.5].

Proposition 3.9.8. *If q is a primitive Lipschitz quaternion with $|q|^2$ odd, one has $\Gamma_{\mathsf{pc}}(R(q)) = \mathrm{Im}(q\mathbb{L})$.*

Proof. From Proposition 3.9.7, we infer that

$$\Gamma_{\mathsf{bcc}}(R(q)) \cap \mathrm{Im}(\mathbb{L}) \,=\, \mathrm{Im}(q\mathbb{J}) \cap \mathrm{Im}(\mathbb{L}).$$

As $\Gamma_{\mathsf{pc}}(R(q)) \subseteq \Gamma_{\mathsf{bcc}}(R(q)) \cap \mathrm{Im}(\mathbb{L})$, and both $\Gamma_{\mathsf{pc}}(R(q))$ and $\Gamma_{\mathsf{bcc}}(R(q)) \cap \mathrm{Im}(\mathbb{L})$ have index 2 in $\Gamma_{\mathsf{bcc}}(R(q))$, we also infer $\Gamma_{\mathsf{pc}}(R(q)) = \Gamma_{\mathsf{bcc}}(R(q)) \cap \mathrm{Im}(\mathbb{L})$. A similar argument applied to $\mathrm{Im}(q\mathbb{L}) \subseteq \mathrm{Im}(q\mathbb{J}) \cap \mathrm{Im}(\mathbb{L})$ shows that one has $\mathrm{Im}(q\mathbb{L}) = \mathrm{Im}(q\mathbb{J}) \cap \mathrm{Im}(\mathbb{L})$, which completes the proof. □

Again, in analogy to the situation for Γ_{bcc}, we can find a quaternion $r \in \mathbb{L}$ such that $\Gamma_{\mathsf{pc}}(R(q)) = \mathrm{Im}(r\mathbb{L})$ if $|q|^2$ is even.

Let us return to the CSLs of Γ_{bcc}. Proposition 3.9.7 shows that any CSL of Γ_{bcc} is the projection $\mathrm{Im}(q\mathbb{J})$ of an ideal $q\mathbb{J}$ of $\mathbb{J}$. On the other hand, whenever q is an odd primitive quaternion, $\mathrm{Im}(q\mathbb{J})$ is a CSL of Γ_{bcc}. If we can show that there is a bijection between the set of ideals $\{q\mathbb{J} \mid q \text{ is primitive and odd}\}$ and the set of CSLs, then we can easily count the CSLs of a given index, as the number of ideals of a fixed index is well known [86]. The first step into this direction is the following result.

Lemma 3.9.9. *Let $q, r \in \mathbb{J}$ such that $|q|^2$ and $|r|^2$ are odd. Then, one has $\mathrm{Im}(q\mathbb{J}) \subseteq \mathrm{Im}(r\mathbb{J})$ if and only if $q\mathbb{J} \subseteq r\mathbb{J}$.*

PROOF. Only the 'only if' part is non-trivial. $\mathrm{Im}(q\mathbb{J}) \subseteq \mathrm{Im}(r\mathbb{J})$ implies that $|r|^2$ divides $|q|^2$. Now,

$$\mathrm{Im}(r\mathbb{J}) \,=\, \mathrm{Im}(r\mathbb{J}) + \mathrm{Im}(q\mathbb{J}) \,=\, \mathrm{Im}(r\mathbb{J} + q\mathbb{J}) \,=\, \mathrm{Im}(s\mathbb{J}),$$

which shows that $|r|^2 = |s|^2$, where s is the greatest common left divisor of r and q. Hence $s^{-1}r \in \mathbb{J}$, but as $|s^{-1}r| = 1$, it must be a unit. Thus $q\mathbb{J} \subseteq s\mathbb{J} = r\mathbb{J}$. □

From this, we infer the following result; compare [12] for a similar result in a more general context.

Corollary 3.9.10. *Let $q, r \in \mathbb{J}$ such that $|q|^2$ and $|r|^2$ are odd. Then, one has $\mathrm{Im}(q\mathbb{J}) = \mathrm{Im}(r\mathbb{J})$ if and only if $q\mathbb{J} = r\mathbb{J}$.* □

In other words, putting the previous steps together, we have proved the following result.

Lemma 3.9.11. *The mapping $q\mathbb{J} \mapsto \Gamma_{\mathsf{bcc}}(R(q))$, which maps the set of left ideals generated by primitive quaternions with $|q|^2$ odd onto the set of CSLs of Γ_{bcc}, is a bijection.* □

An analogous result can be proved for the other cubic lattices as well.

Theorem 3.9.12. *The mapping $q\mathbb{J} \mapsto \Gamma_a(R(q)) = \mathrm{Im}(q\mathbb{J}) \cap \Gamma_a$, with fixed type $a \in \{\mathsf{pc}, \mathsf{bcc}, \mathsf{fcc}\}$, defines a bijection between the set of left ideals generated by primitive quaternions with $|q|^2$ odd and the set of CSLs of Γ_a.*

PROOF. From $\Gamma_a(R(q)) \subseteq \Gamma_a$ and $\Gamma_a(R(q)) \subseteq \Gamma_{\mathsf{bcc}}(R(q)) = \mathrm{Im}(q\mathbb{J})$, we see that $\Gamma_a(R(q)) \subseteq \mathrm{Im}(q\mathbb{J}) \cap \Gamma_a$. As $[\Gamma_{\mathsf{bcc}} : \Gamma_a]$ is a power of 2 and the coincidence indices are always odd, index considerations show that we even have $\Gamma_a(R(q)) = \mathrm{Im}(q\mathbb{J}) \cap \Gamma_a$. Now, the theorem is a consequence of the bijection in Lemma 3.9.11, where index considerations confirm that $\mathrm{Im}(q\mathbb{J}) = \mathrm{Im}(q'\mathbb{J})$ holds if and only if $\mathrm{Im}(q\mathbb{J}) \cap \Gamma_a = \mathrm{Im}(q'\mathbb{J}) \cap \Gamma_a$. □

So far, we get the following result for the arithmetic functions that count the number of CSLs and coincidence isometries for a given index, where we use $c_{\mathsf{bcc}}(n) := c_{\Gamma_{\mathsf{bcc}}}(n)$ for simplicity.

Corollary 3.9.13. *For the cubic lattices according to Eq.* (3.9.1)*, one has*

$$c^{\mathsf{iso}}_{\mathsf{bcc}}(n) = c_{\mathsf{bcc}}(n) \,=\, c^{\mathsf{iso}}_{\mathsf{pc}}(n) \,=\, c_{\mathsf{pc}}(n) \,=\, c^{\mathsf{iso}}_{\mathsf{fcc}}(n) \,=\, c_{\mathsf{fcc}}(n).$$

PROOF. It follows from Theorem 3.9.12 that the number of CSLs of any cubic lattice for a given index is given by the number of left ideals generated by primitive q with $|q|^2$ odd, hence $c_{\mathsf{bcc}}(n) = c_{\mathsf{pc}}(n) = c_{\mathsf{fcc}}(n)$. As the coincidence

indices of a given coincidence isometry are the same for all cubic lattices, we also have $c^{\mathsf{iso}}_{\mathsf{bcc}}(n) = c^{\mathsf{iso}}_{\mathsf{pc}}(n) = c^{\mathsf{iso}}_{\mathsf{fcc}}(n)$.

It remains to show $c_{\mathsf{bcc}}(n) = c^{\mathsf{iso}}_{\mathsf{bcc}}(n)$. By Section 3.7.4, $c^{\mathsf{iso}}(n) = c^{\mathsf{rot}}(n)$ holds for any lattice in odd dimensions and for any $n \in \mathbb{N}$. It thus suffices to show that $c_{\mathsf{bcc}}(n) = c^{\mathsf{rot}}_{\mathsf{bcc}}(n)$. Recall that any coincidence rotation can be parametrised either by an odd primitive quaternion q or by a primitive quaternion $q(1+\mathrm{i})$, where q is again odd. As the rotation $R(1+\mathrm{i})$ is a symmetry operation of all three cubic lattices, q and $q(1+\mathrm{i})$ generate the same CSL. As all symmetry rotations are generated by quaternions u or $(1+\mathrm{i})u$, where u is a unit, Theorem 3.9.12 implies $c_{\mathsf{bcc}}(n) = c^{\mathsf{rot}}_{\mathsf{bcc}}(n) = c^{\mathsf{iso}}_{\mathsf{bcc}}(n)$. □

Actually, we can calculate $c_{\varGamma}(n)$ explicitly. We first note that $c_{\varGamma}(n)$ is multiplicative, as $\mathbb{J}$ is a principal ideal ring and thus has an essentially unique prime factorisation. Let us recall that uniqueness is a bit subtle here, since $\mathbb{J}$ is not Abelian, and the prime factorisation depends on the ordering of the factors in general. But, if we fix an ordering (by requiring that the norm of the prime factors should increase monotonically, say), the prime factors are unique up to units. Thus, $c_{\varGamma}(n)$ is determined by its values for prime powers, and, in particular, we have

$$c_{\mathsf{bcc}}(p^r) \,=\, (p+1)\,p^{r-1} \tag{3.9.3}$$

if p is an odd prime, as $c_{\mathsf{bcc}}(p^r)$ is the number of primitive ideals of norm p^{2r}; see [58, Ch. 10]. Furthermore, note that $24\,c_{\mathsf{bcc}}(p^r)$ is the number of primitive quaternions of norm p^r and $8\,c_{\mathsf{bcc}}(p^r)$ is the number of primitive representations of p^r as a sum of four squares, which follows easily from the total number of representations; compare [51, 54]. Thus, $8c_{\mathsf{bcc}}(m)$ is the number of primitive representations of m as a sum of four squares, if m is odd,[10] and $c_{\mathsf{bcc}}(m) = 0$ for m even. Hence, we obtain an explicit expression for the generating function; see also [4] and [12, Sec. 2].

Theorem 3.9.14 ([4, Props. 3.2 and 3.3])**.** *For any cubic lattice $\varGamma \subset \mathbb{R}^3$ in the setting of Eq.* (3.9.1)*, we have*

$$\mathrm{OC}(\varGamma) \,=\, \mathrm{OS}(\varGamma) \,=\, \mathrm{OC}(\varGamma_{\mathsf{bcc}}) \,=\, \mathrm{O}(3,\mathbb{Q}).$$

In particular, if q is a primitive Hurwitz quaternion and ℓ is the maximal exponent such that $2^{\ell}\big||q|^2$, then the coincidence index is given by

$$\varSigma_{\varGamma}(R(q)) \,=\, \varSigma_{\mathsf{bcc}}(R(q)) \,=\, \mathrm{den}_{\varGamma}(R(q)) \,=\, \frac{|q|^2}{2^{\ell}}.$$

[10] This is part of Jacobi's four-square theorem [51], which states that the number of ways to represent m as the sum of four squares is 8 times the sum of its divisors (if m is odd) and 24 times the sum of its odd divisors (if m is even).

Moreover, we have $\Psi_{\Gamma}(s) = \Psi_{\Gamma}^{\mathsf{iso}}(s) = \Psi_{\mathsf{bcc}}(s)$*, which is given by the equation*

$$\begin{aligned}\Psi_{\mathsf{bcc}}(s) &= \sum_{m=1}^{\infty} \frac{c_{\Gamma}(m)}{m^s} = \prod_{p\neq 2} \frac{1+p^{-s}}{1-p^{1-s}} \\ &= \frac{1}{1+2^{-s}}\, \frac{\zeta_{\mathbb{J}}(s/2)}{\zeta(2s)} = \frac{1-2^{1-s}}{1+2^{-s}}\, \frac{\zeta(s)\,\zeta(s-1)}{\zeta(2s)} \\ &= 1 + \tfrac{4}{3^s} + \tfrac{6}{5^s} + \tfrac{8}{7^s} + \tfrac{12}{9^s} + \tfrac{12}{11^s} + \tfrac{14}{13^s} + \tfrac{24}{15^s} + \tfrac{18}{17^s} + \tfrac{20}{19^s} + \tfrac{32}{21^s} + \cdots ,\end{aligned}$$

where all positive odd integers appear in the denominator. □

Here, we have made use of the zeta function $\zeta_{\mathbb{J}}$ of the Hurwitz ring from Eq. (3.5.21), which counts the non-trivial left ideals of $\mathbb{J}$. We observe that $\zeta_{\mathbb{J}}(s)$ and $\Psi_{\mathsf{bcc}}(s)$ differ by the factors $\frac{1}{1+2^{-s}}$ and $\frac{1}{\zeta(2s)}$. Note that the term $(1+2^{-s})\,\zeta(2s)$ is the generating function for the two-sided ideals of $\mathbb{J}$. But as the two-sided ideals only generate the trivial CSL $\Gamma(R) = \Gamma$, they do not contribute to $\Psi_{\mathsf{bcc}}(s)$, hence their contribution to $\zeta_{\mathbb{J}}(s)$ has to be factored out to obtain $\Psi_{\mathsf{bcc}}(s)$.

It follows from the properties of Riemann's zeta function that $\Psi_{\mathsf{bcc}}(s)$ is a meromorphic function of s. In particular, Ψ_{bcc} is analytic in the half-plane $\{\mathrm{Re}(s) \geqslant 2\}$, and its rightmost pole is located at $s = 2$. Using Delange's theorem (Theorem 3.4.1), we find the asymptotic growth behaviour (compare [4] and [12, Sec. 2])

$$\sum_{n\leqslant x} c_{\mathsf{bcc}}(n) = \frac{3x^2}{\pi^2} + \mathcal{O}(x^2)\,, \qquad \text{as } x \to \infty. \tag{3.9.4}$$

In contrast to the CSLs of the square and the triangular lattice in the plane, the CSLs of the cubic lattice generally fail to be similar sublattices, and usually have lower symmetries; see [92] for details.

Remark 3.9.15. It is an interesting question what kind of grain boundaries are compatible with CSLs of cubic lattices, as the geometric situation in 3-space is certainly richer than in the plane. Now, a large number of CSLs for cubic lattices can be written as $\Gamma(R)$, where R is actually a rotation through π around an axis in a lattice direction v. These are precisely the rotations parametrised by a quaternion $q = (0, v)$; compare [45].

The lattice planes perpendicular to v through a point nv with $n \in \mathbb{Z}$ are invariant under a rotation about v through π. Any of these can act as a defect-free (or perfect) grain boundary between two crystal halves, and the entire configuration appears as a stacking fault; see Figure 3.9.1 for an illustration of a stacking sequence that corresponds to a CSL with index $\Sigma = 3$ and hexagonal symmetry. Note that the order of the layers is reversed in the rotated half.

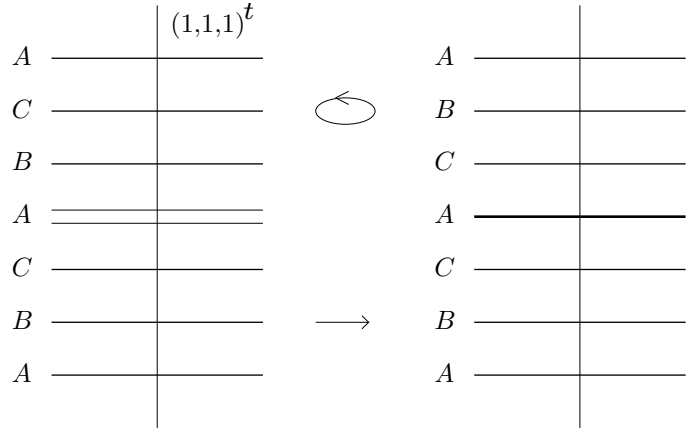

FIGURE 3.9.1. Sketch of a stacking fault in a cubic crystal. The upper half is rotated through an angle π about the $(1,1,1)^t$-axis. This keeps the A layers fixed and interchanges layers of types B and C.

In contrast to cubic lattices, a rotation R through π about a lattice vector v is not necessarily a coincidence rotation for a general lattice. However, if R is a coincidence rotation, the corresponding lattice planes orthogonal to v are invariant under R, and analogous stacking faults may occur.

Apart from their obvious relevance to the twinning structure of cubic crystals, coincidence isometries in the form of rotations through π or simple reflections are useful generators for more complicated coincidence isometries in higher dimensions. In fact, this leads to one of the few approaches to higher dimensions known so far; see Section 3.13 below for more. ♢

Remark 3.9.16. The results for the cubic lattices can be generalised to certain embedded $\mathbb{Z}$-modules of the form $\mathrm{Im}(\mathcal{O})$, where $\mathcal{O}$ is a maximal order in a quaternion algebra [12]. The situation is quite convenient in the case of quaternion algebras $\mathbb{H}(K)$ over a real algebraic number field K such that both K and $\mathbb{H}(K)$ have class number 1. In particular, apart from the Hurwitz ring $\mathbb{J}$, this includes the icosian ring $\mathbb{I} \subset \mathbb{H}(\mathbb{Q}(\sqrt{5}\,))$ and the cubian ring $\mathbb{K} \subset \mathbb{H}(\mathbb{Q}(\sqrt{2}\,))$; see [11, 12] for details.

The counterpart to the odd primitive quaternions are the so-called $\mathcal{O}$-reduced quaternions. If q is $\mathcal{O}$-reduced, many of our results for the cubic lattices can be reformulated for $\mathcal{O} \subset \mathbb{H}(K)$. In particular, the coincidence index is given by $\Sigma_{\mathcal{O}}(R(q)) = N(|q|^2)$, where N is the norm in the number field K; compare [12, Prop. 5]. This follows from the explicit expression for the CSMs

$$\mathrm{Im}(\mathcal{O}) \cap \mathrm{Im}(q\mathcal{O}q^{-1}) \;=\; \mathrm{Im}(\mathcal{O} \cap q\mathcal{O}q^{-1}) \;=\; \mathrm{Im}(q\mathcal{O});$$

compare [12, Lemmas 4, 5 and 6]. Moreover, there still is a bijection between the CSMs $\mathrm{Im}(q\mathcal{O})$ and the left ideals $q\mathcal{O}$; see [12, Thm. 1]. This makes it possible to count the CSMs and to write down an explicit expression for the generating function [12, Thm. 2], namely

$$\Psi_{\mathcal{O}}^{\mathsf{iso}}(s) \,=\, \Psi_{\mathcal{O}}(s) \,=\, \frac{\zeta_{\mathcal{O}}(s/2)}{\zeta_{\mathcal{O}.\mathcal{O}}(s/2)} \,=\, E(s)\frac{\zeta_K(s)\,\zeta_K(s-1)}{\zeta_K(2s)}.$$

Here, $\zeta_{\mathcal{O}}(s)$ and $\zeta_{\mathcal{O}.\mathcal{O}}(s)$ denote the zeta functions of the left and the two-sided ideals of $\mathcal{O}$, respectively, whereas $\zeta_K(s)$ is the zeta function of K and $E(s)$ is either 1 or an additional analytic factor that takes care of the extra contributions from (finitely many) ramified primes. As a consequence, one gets the asymptotic behaviour [12, Cor. 1]

$$\sum_{n\leqslant x} c_{\mathcal{O}}(n) \,\sim\, \rho_{\mathcal{O}}\frac{x^2}{2}\,, \qquad \text{as } x\to\infty$$

for some $\rho_{\mathcal{O}} \in \mathbb{R}_+$. ◊

3.10. The four-dimensional hypercubic lattices

Let us continue with some examples in 4-space, and let us start with the hypercubic lattices. So far, in all our examples, the generating functions for the number of coincidence rotations (modulo symmetries) and the number of CSLs coincided, as two different coincidence rotations generated the same CSL if and only if they were symmetry related. This is no longer the case in the examples to come.

3.10.1. The centred hypercubic lattice D_4^*

As we have already seen in Section 3.5.5, any similarity rotation can be parametrised by a pair of $\mathbb{J}$-primitive Hurwitz quaternions, where $\mathbb{J} = D_4^*$ as lattices in our setting. In fact, it follows from Corollary 3.7.28 and Eq. (3.5.23) that $R = R(p,q)$ is a coincidence rotation of $\mathbb{J}$ if and only if $|pq| \in \mathbb{N}$. A pair $(p,q) \in \mathbb{J}\times\mathbb{J}$ with $|pq| \in \mathbb{N}$ is called *admissible*. Thus, $R(p,q)$ is a coincidence rotation of $\mathbb{J}$ if and only if $R(p,q)$ can be parametrised by an admissible pair of $\mathbb{J}$-primitive Hurwitz quaternions. As a consequence, we have the following result.

Fact 3.10.1. $\mathrm{SOC}(\mathbb{J}) = \mathrm{SO}(4,\mathbb{Q})$. □

However, it turns out that primitive quaternions are not an optimal choice in this case, and we prefer a suitably scaled pair. To find such a pair, note first that $|pq|^2$ is a square in $\mathbb{N}$ for any admissible pair, and so is

$|pq|^2/\gcd(|p|^2,|q|^2)^2$. As the two factors

$$\frac{|q|^2}{\gcd(|p|^2,|q|^2)} \quad \text{and} \quad \frac{|p|^2}{\gcd(|p|^2,|q|^2)}$$

are coprime, they must be squares as well. Hence, we can define the (coprime) integers

$$\alpha_p := \sqrt{\frac{|q|^2}{\gcd(|p|^2,|q|^2)}} \quad \text{and} \quad \alpha_q := \sqrt{\frac{|p|^2}{\gcd(|p|^2,|q|^2)}}. \tag{3.10.1}$$

Of course, $(x,y) = (\alpha_p p, \alpha_q q)$ defines the same rotation as (p,q). However, we can deal more easily with (x,y) since $|x|^2 = |y|^2$. Moreover, the octuple $(x,y) = (\alpha_p p, \alpha_q q)$ is primitive for primitive p and q, in the sense that $\frac{1}{n}(\alpha_p p, \alpha_q q) \in \mathbb{J}\times\mathbb{J}$ if and only if $n \in \{\pm 1\}$. This guarantees that there exist quaternions $v, w \in \mathbb{J}$ such that $\langle x|v\rangle + \langle y|w\rangle = 1$. We shall call a pair of quaternions with these two properties an *extended admissible pair*, and denote it by $(p_\alpha, q_\alpha) = (\alpha_p p, \alpha_q q)$.

Clearly, scaling quaternions does not change the rotation $R(p,q)$. On the other hand, there are a lot of rotations that yield the same CSL, namely all rotations that only differ by a symmetry operation of $\mathbb{J}$. Let us denote the corresponding group by

$$\mathrm{SO}(\mathbb{J}) := \{R \in \mathrm{SO}(4,\mathbb{R}) \mid R\mathbb{J} = \mathbb{J}\},$$

which is a group of order $24^2 = 576$. Recall that we call two coincidence rotations R, R' symmetry related if there exists an $S \in \mathrm{SO}(\mathbb{J})$ such that $R' = RS$ holds.

Let us have a closer look at symmetry-related rotations. It follows from $R(p,q)\mathbb{J} = \frac{1}{|pq|} p\mathbb{J}\bar{q}$ that $R(p,q)\mathbb{J} = R(p',q')\mathbb{J}$ if and only if

$$\frac{1}{|pp'|}\bar{p}p'\mathbb{J} = \frac{1}{|qq'|}\mathbb{J}\bar{q}q'.$$

This means that (p,q) and (pr,qr) are symmetry related if and only if r is a quaternion such that $r\mathbb{J}$ is a two-sided ideal. Apart from scaling factors and units, the only non-trivial such quaternion is $r = 1 + \mathrm{i}$; see [86, 60, 35, 58]. Thus, $R(p,q)\mathbb{J} = R(pr,qr)\mathbb{J}$, and, as r is the only prime quaternion (up to units) of norm $|r|^2 = 2$, we can find, for any rotation $R \in \mathrm{SOC}(\mathbb{J})$, a pair of quaternions (p,q) with $|p|^2$ and $|q|^2$ odd such that R is symmetry related to $R(p,q)$. We can thus confine our considerations to the latter rotations, and we will call an extended admissible pair (p,q) with $|p|^2$ and $|q|^2$ odd an *odd extended admissible* pair.

In fact, we can express all CSLs in terms of odd extended admissible pairs as follows.

Lemma 3.10.2. *If (p,q) is an odd extended admissible pair, one has*

$$p\mathbb{J}+\mathbb{J}\bar{q} \subseteq \mathbb{J}\cap\frac{p\mathbb{J}\bar{q}}{|pq|}.$$

PROOF. Clearly, $p\mathbb{J}\subseteq\mathbb{J}$ and $\mathbb{J}\bar{q}\subseteq\mathbb{J}$, thus giving $p\mathbb{J}+\mathbb{J}\bar{q}\subseteq\mathbb{J}$. On the other hand, since $|p|^2=|q|^2$, one has

$$p\mathbb{J} = \frac{p\mathbb{J}q\bar{q}}{|q|^2} \subseteq \frac{p\mathbb{J}\bar{q}}{|q|^2} = \frac{p\mathbb{J}\bar{q}}{|pq|}, \tag{3.10.2}$$

and a similar argument for $\mathbb{J}\bar{q}$ yields $p\mathbb{J}+\mathbb{J}\bar{q}\subseteq\frac{p\mathbb{J}\bar{q}}{|pq|}$. □

The first step for the converse inclusion is the following result, where we return to the more general case of extended admissible pairs for a moment.

Lemma 3.10.3. *If (p,q) is an extended admissible pair, one has*

$$2\left(\mathbb{J}\cap\frac{p\mathbb{J}\bar{q}}{|pq|}\right) \subseteq p\mathbb{J}+\mathbb{J}\bar{q}.$$

PROOF. Let $x\in\mathbb{J}\cap\frac{p\mathbb{J}\bar{q}}{|pq|}$. Then, there exists a $y\in\mathbb{J}$ such that $x=\frac{py\bar{q}}{|pq|}$. Since (p,q) is an extended admissible pair, there exist quaternions $v,w\in\mathbb{J}$ such that $\langle p|v\rangle+\langle q|w\rangle=1$. Consequently,

$$\begin{aligned}2x &= 2\big(\langle p|v\rangle+\langle q|w\rangle\big)x = 2\langle p|v\rangle x+2x\langle q|w\rangle = p\bar{v}x+v\bar{p}x+xq\bar{w}+xw\bar{q}\\ &= p\bar{v}x+vy\bar{q}+py\bar{w}+xw\bar{q} \in p\mathbb{J}+\mathbb{J}\bar{q},\end{aligned}$$

where we have made use of the identity $\langle a|b\rangle=\frac{1}{2}(a\bar{b}+b\bar{a})$. □

Trivially, since $|p|^2=|q|^2$, one has

$$|p|^2\left(\mathbb{J}\cap\frac{p\mathbb{J}\bar{q}}{|pq|}\right) = |p|^2\mathbb{J}\cap p\mathbb{J}\bar{q} \subseteq p\mathbb{J}+\mathbb{J}\bar{q}.$$

If we restrict again to odd extended admissible pairs, we get

$$\mathbb{J}\cap\frac{p\mathbb{J}\bar{q}}{|pq|} = 2\left(\mathbb{J}\cap\frac{p\mathbb{J}\bar{q}}{|pq|}\right)+|p|^2\left(\mathbb{J}\cap\frac{p\mathbb{J}\bar{q}}{|pq|}\right)\subseteq p\mathbb{J}+\mathbb{J}\bar{q},$$

since $|p|^2$ is odd. Hence, we have proved the following result.

Theorem 3.10.4. *Let (p,q) be an odd extended admissible pair. Then,*

$$\mathbb{J}\cap\frac{p\mathbb{J}\bar{q}}{|pq|} = p\mathbb{J}+\mathbb{J}\bar{q},$$

so each CSL of the centred hypercubic lattice is of the form $p\mathbb{J}+\mathbb{J}\bar{q}$ for a suitable odd extended admissible pair. □

This explicit expression of the CSLs of $\mathbb{J}$ in terms of a sum of ideals of $\mathbb{J}$ is very useful, as it does not only help to calculate their indices, but it also allows us to determine which coincidence rotations yield the same CSL.

Let us first state the result for the index.

Theorem 3.10.5 ([97, Theorem 4.1.6])**.** *If (p, q) is an odd extended admissible pair, one has $\Sigma(R(p,q)) = |p|^2$.*

SKETCH OF PROOF. The idea of the proof is to exploit the equation

$$p\mathbb{J} \subseteq p\mathbb{J} + \mathbb{J}\bar{q} = \mathbb{J} \cap \frac{p\mathbb{J}\bar{q}}{|pq|} \subseteq \mathbb{J}$$

to show $\Sigma(R(\bar{p},q))\Sigma(R(p,q)) = |p|^4$. By proving that the index $\Sigma(R(p,q))$ divides $|p|^2$, one then infers $\Sigma(R(p,q)) = |p|^2$. For the rather technical details, we refer to [97]. □

Remark 3.10.6. It may be useful to formulate the index in terms of primitive admissible pairs. Let p, q be primitive odd quaternions with associated extended pair $(p_\alpha, q_\alpha) = (\alpha_p p, \alpha_q q)$. Then,

$$\begin{aligned}\Sigma(R(p,q)) &= \alpha_p^2\,|p|^2 = \alpha_q^2\,|q|^2 = \alpha_p\alpha_q\,|pq| \\ &= \operatorname{lcm}\bigl(|p|^2,|q|^2\bigr) = \alpha_p^2\alpha_q^2\gcd\bigl(|p|^2,|q|^2\bigr).\end{aligned}$$

Note that $|pq|$ is the denominator of $R(p,q)$. This shows that, in general, $\operatorname{den}(R)$ and $\Sigma(R)$ do *not* coincide for the lattice D_4^*, which is in contrast to the three-dimensional cubic lattices. In fact, $\operatorname{den}(R) = \Sigma(R)$ holds if and only if $\alpha_p = \alpha_q = 1$. ◊

Remark 3.10.7. This explicit expression for the coincidence indices allows us to determine the coincidence spectrum. As in Remark 3.9.6, we conclude that $|p|^2$ and $|q|^2$ run through all odd positive integers, and the possible coincidence indices thus are exactly the odd positive integers. In other words, the coincidence spectrum of D_4^* and D_4, which we know to be similar lattices, is the set of all odd positive integers,

$$\Sigma\bigl(\mathrm{SOC}(D_4^*)\bigr) = \Sigma\bigl(\mathrm{SOC}(D_4)\bigr) = 2\mathbb{N}_0 + 1.$$

This is exactly the same spectrum we have found for the three-dimensional cubic lattices; compare Remark 3.9.6. As D_4^* has reflections among its symmetry operations, this is also the full spectrum $\Sigma\bigl(\mathrm{OC}(D_4^*)\bigr) = \Sigma\bigl(\mathrm{SOC}(D_4^*)\bigr)$ by Remark 3.7.8. ◊

Our next task is to enumerate the coincidence isometries of D_4^*. Since the point group of D_4^* contains $24^2 = 576$ rotations, the number of coincidence rotations of a given index n can be written as $576\,c_{D_4^*}^{\mathsf{rot}}(n)$. As the point group contains also reflections, the number of coincidence isometries is twice this number, $1152\,c_{D_4^*}^{\mathsf{rot}}(n)$.

By Theorem 3.10.5, counting the number of coincidence rotations is equivalent to counting the number of odd extended admissible pairs. We first observe that $c_{D_4^*}^{\mathsf{rot}}(n)$ is a multiplicative function, which follows from the essentially unique prime factorisation in $\mathbb{J}$. Indeed, if (p, q) and (r, s) are

odd extended admissible pairs with $|p|^2 = m$ and $|r|^2 = n$ for m, n coprime, (pr, qs) is an odd extended admissible pair with $|pr|^2 = mn$. Conversely, any odd extended admissible pair (p, q) with $|p|^2 = mn$ can be decomposed into odd extended admissible pairs with index m and n, respectively. As this decomposition is unique up to units, multiplicativity follows.

Thus, we only need to compute $c^{\mathsf{rot}}_{D_4^*}(n)$ for n being a prime power. In the following, let π denote a rational prime (we choose π here as we have used p for quaternions already). As odd extended admissible pairs consist of odd quaternions only, $c^{\mathsf{rot}}_{D_4^*}(2^r) = 0$. Hence, π is always odd in what follows. It is now a purely combinatorial task to determine $c^{\mathsf{rot}}_{D_4^*}(\pi^r)$. The number of primitive quaternions p with norm $|p|^2 = \pi^r$ is given by $24 f(\pi^r)$ with $f(\pi^r) = (\pi+1)\pi^{r-1}$ for $r \geqslant 1$; compare Eq. (3.9.3). Any odd extended admissible pair (p, q) with $|p|^2 = \pi^r$ can be obtained from a primitive admissible pair (p_1, q_1) with $|p_1|^2 = \pi^{r'}$, $|q_1|^2 = \pi^{r''}$, $r = \max(r', r'')$, and $r' - r''$ even. Hence,

$$\begin{aligned} c^{\mathsf{rot}}_{D_4^*}(\pi^r) \;&=\; f(\pi^r)^2 + 2\sum_{s=1}^{[r/2]} f(\pi^r)\, f(\pi^{r-2s}) \\ &=\; \frac{\pi+1}{\pi-1}\,\pi^{r-1}\,(\pi^{r+1} + \pi^{r-1} - 2). \end{aligned} \tag{3.10.3}$$

Let us summarise this result in the following theorem, where we change the notation and use p to denote a rational prime.

Theorem 3.10.8. *The number of coincidence rotations of D_4^* of index n is given by $576\, c^{\mathsf{rot}}_{D_4^*}(n)$, where $c^{\mathsf{rot}}_{D_4^*}(n)$ is a multiplicative arithmetic function. It is determined by $c^{\mathsf{rot}}_{D_4^*}(2^r) = 0$ for $r \geqslant 1$ together with*

$$c^{\mathsf{rot}}_{D_4^*}(p^r) \;=\; \frac{p+1}{p-1}\,p^{r-1}\,(p^{r+1} + p^{r-1} - 2)$$

if p is an odd prime and $r \geqslant 1$. □

The multiplicativity of $c^{\mathsf{rot}}_{D_4^*}(n)$ guarantees that the corresponding Dirichlet series generating function can be written as an Euler product,

$$\begin{aligned} \Psi^{\mathsf{rot}}_{D_4^*}(s) \;&=\; \sum_{n=1}^{\infty} \frac{c^{\mathsf{rot}}_{D_4^*}(n)}{n^s} \;=\; \prod_{p\neq 2} \frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \\ &=\; \frac{1-2^{1-s}}{1+2^{-s}}\,\frac{1-2^{2-s}}{1+2^{1-s}}\,\frac{\zeta(s)\,\zeta(s-1)^2\,\zeta(s-2)}{\zeta(2s)\,\zeta(2s-2)}, \end{aligned} \tag{3.10.4}$$

where the first few terms read as follows,

$$\Psi^{\mathsf{rot}}_{D_4^*}(s) = 1 + \tfrac{16}{3^s} + \tfrac{36}{5^s} + \tfrac{64}{7^s} + \tfrac{168}{9^s} + \tfrac{144}{11^s} + \tfrac{196}{13^s} + \tfrac{576}{15^s} + \tfrac{324}{17^s} + \tfrac{400}{19^s} + \tfrac{1024}{21^s} + \cdots$$

It is remarkable that $\Psi^{\mathsf{rot}}_{D_4^*}(s)$ can be expressed in terms of the cubic generating function $\Psi_{\mathsf{bcc}}(s)$ from Theorem 3.9.14, which follows immediately

from its explicit expression in terms of zeta functions from Eq. (3.10.4). In particular, one has

$$\Psi^{\mathsf{rot}}_{D_4^*}(s) \;=\; \Psi_{\mathsf{bcc}}(s)\Psi_{\mathsf{bcc}}(s-1). \tag{3.10.5}$$

This explicit expression shows that $\Psi^{\mathsf{rot}}_{D_4^*}(s)$ is a meromorphic function in the complex plane. Its rightmost pole is at $s = 3$, with residue $\frac{630}{\pi^6}\zeta(3)$. Using Theorem 3.4.1, we obtain the asymptotic behaviour

$$\sum_{n\leqslant x} c^{\mathsf{rot}}_{D_4^*}(n) \;\sim\; \frac{210}{\pi^6}\zeta(3)\, x^3 \;\approx\; 0.262570\, x^3$$

as $x \to \infty$.

Next, we want to calculate the number $c_{D_4^*}(n)$ of distinct CSLs of a given index n. In contrast to the three-dimensional cubic lattices, where we have $c^{\mathsf{rot}}(n) = c(n)$, it turns out that $c_{D_4^*}(n)$ and $c^{\mathsf{rot}}_{D_4^*}(n)$ generally differ. Clearly, we have the upper bound $c_{D_4^*}(n) \leqslant c^{\mathsf{rot}}_{D_4^*}(n)$. To calculate $c_{D_4^*}(n)$, we must determine which coincidence rotations generate the same CSL.

One knows from Lemma 3.7.33 that two CSLs can only agree if the corresponding coincidence indices are the same. In addition, the denominators of the inverses must be equal, but as $\mathrm{den}(R) = \mathrm{den}(R^{-1})$, we infer that the denominators must be the same as well. However, these conditions are not yet sufficient. In fact, we need additional conditions, which are a bit technical; compare [14] and see [97, Thm. 4.1.12] for a proof.

Theorem 3.10.9. *Let (q_1, p_1) and (q_2, p_2) be two primitive admissible pairs of odd quaternions. Then,*

$$\mathbb{J} \cap \frac{p_1 \mathbb{J} \bar{q}_1}{|p_1 q_1|} \;=\; \mathbb{J} \cap \frac{p_2 \mathbb{J} \bar{q}_2}{|p_2 q_2|}$$

holds if and only if the following conditions are satisfied (up to units):

(1) $|p_1 q_1| = |p_2 q_2|$,
(2) $\mathrm{lcm}\big(|p_1|^2, |q_1|^2\big) = \mathrm{lcm}\big(|p_2|^2, |q_2|^2\big)$,
(3) $\mathrm{gcld}\big(p_1, |p_1 q_1|\big) = \mathrm{gcld}\big(p_2, |p_2 q_2|\big)$, *and*
(4) $\mathrm{gcld}\big(q_1, |p_1 q_1|\big) = \mathrm{gcld}\big(q_2, |p_2 q_2|\big)$. □

Note that the first two conditions correspond to the aforementioned condition that the coincidence indices and the denominator are the same (recall from Remark 3.10.6 that $\Sigma(R(p,q)) = \mathrm{lcm}(|p|^2, |q|^2)$ and $\mathrm{den}(R(p,q)) = |pq|$, if (p, q) is a primitive admissible pair of odd quaternions).

Remark 3.10.10. One gets an equivalent set of conditions for the equality of two CSLs if one replaces conditions (1) and (2) in Theorem 3.10.9 by $|p_1|^2 = |p_2|^2$ and $|q_1|^2 = |q_2|^2$. It is obvious that the two conditions $|p_1|^2 = |p_2|^2$ and $|q_1|^2 = |q_2|^2$ imply that the denominators $|p_1 q_1| = |p_2 q_2|$ and the

coincidence indices $\operatorname{lcm}(|p_1|^2,|q_1|^2) = \operatorname{lcm}(|p_2|^2,|q_2|^2)$ are the same. The reverse direction is more complicated, as the two conditions $|p_1q_1| = |p_2q_2|$ and $\operatorname{lcm}(|p_1|^2,|q_1|^2) = \operatorname{lcm}(|p_2|^2,|q_2|^2)$ alone only yield $\gcd(|p_1|^2,|q_1|^2) = \gcd(|p_2|^2,|q_2|^2)$, but not $|p_1|^2 = |p_2|^2$ and $|q_1|^2 = |q_2|^2$ directly. In fact, we need both of the other two conditions, $\gcd(p_1,|p_1q_1|) = \gcd(p_2,|p_2q_2|)$ and $\gcd(q_1,|p_1q_1|) = \gcd(q_2,|p_2q_2|)$, to establish $|p_1|^2 = |p_2|^2$ and $|q_1|^2 = |q_2|^2$ as well; compare [97, Proof of Thm. 4.1.12 and Rem. 4.1.13]. ◊

We are now ready to count the number $c_{D_4^*}(n)$ of CSLs. It follows from Theorem 3.7.18 that $c_{D_4^*}(n)$ is multiplicative, since $c^{\mathsf{iso}}_{D_4^*}(n)$ is multiplicative. As there are no CSLs of even index, $c_{D_4^*}(n)$ is completely determined by $c_{D_4^*}(\pi^r)$ for odd rational primes π and $r \in \mathbb{N}$. The latter can be calculated by counting the number of odd primitive admissible pairs that satisfy the conditions in Theorem 3.10.9 or in Remark 3.10.10. Thus,

$$c_{D_4^*}(\pi^r) \;=\; f(\pi^r)^2 + 2\sum_{s=1}^{[r/2]} f(\pi^{r-s})f(\pi^{r-2s}), \tag{3.10.6}$$

where $f(\pi^r) = (\pi+1)\,\pi^{r-1}$ for $r \geqslant 1$ as above. Note that this expression is very similar to Eq. (3.10.3), the only difference being that one factor $f(\pi^r)$ is replaced by $f(\pi^{r-s})$, where the latter counts the number of distinct $\gcd(p,|pq|)$ with $|p|^2 = \pi^r$ and $|q|^2 = \pi^{r-2s}$.

Evaluating the sum yields the following result, where we again switch to p to denote a rational prime.

Theorem 3.10.11. *The number of distinct CSLs of D_4^* of index n is given by $c_{D_4^*}(n)$. Here, $c_{D_4^*}(n)$ is a multiplicative arithmetic function, which is completely determined by $c_{D_4^*}(2^r) = 0$ for $r \geqslant 1$ together with*

$$c_{D_4^*}(p^r) = \begin{cases} \frac{(p+1)^2}{p^3-1}\big(p^{2r+1} + p^{2r-2} - 2p^{\frac{r-1}{2}}\big), & \text{if } r \geqslant 1 \text{ is odd,} \\ \frac{(p+1)^2}{p^3-1}\big(p^{2r+1} + p^{2r-2} - 2\frac{p^2+1}{p+1}p^{\frac{r-2}{2}}\big), & \text{if } r \geqslant 2 \text{ is even,} \end{cases}$$

for odd primes p. Then,

$$\begin{aligned}\Psi_{D_4^*}(s) = \sum_{n=1}^{\infty}\frac{c_{D_4^*}(n)}{n^s} &= \prod_{p\neq 2}\frac{1+p^{-s}+2p^{1-s}+2p^{-2s}+p^{1-2s}+p^{1-3s}}{(1-p^{2-s})(1-p^{1-2s})} \\ &= 1 + \tfrac{16}{3^s} + \tfrac{36}{5^s} + \tfrac{64}{7^s} + \tfrac{152}{9^s} + \tfrac{144}{11^s} + \tfrac{196}{13^s} + \tfrac{576}{15^s} + \tfrac{324}{17^s} + \tfrac{400}{19^s} + \tfrac{1024}{21^s} + \cdots\end{aligned}$$

is the corresponding Dirichlet series. □

Unfortunately, unlike before, there is no nice representation of $\Psi_{D_4^*}(s)$ as a product of zeta functions. Nevertheless, we can use Theorem 3.4.1 to calculate the asymptotic behaviour as follows.

Note that $\Psi_{D_4^*}(s)$ is quite similar to $\Psi^{\mathsf{rot}}_{D_4^*}(s)$; compare Eq. (3.10.4). In fact, differences between the corresponding counting functions occur only for those integers that are divisible by the square of an odd prime. Thus, the rightmost pole of $\Psi_{D_4^*}(s)$ is still at $s = 3$, which is the same as for $\Psi^{\mathsf{rot}}_{D_4^*}(s)$. This implies the asymptotic behaviour $\sum_{n\leqslant x} c_{D_4^*}(n) \sim cx^3$ as $x \to \infty$ for some positive constant c. To be more specific, we consider the ratio

$$\frac{\Psi_{D_4^*}(s)}{\Psi^{\mathsf{rot}}_{D_4^*}(s)} = \prod_{p\neq 2}\left(1 - \frac{2(p^2-1)p^{-2s}}{(1+p^{-s})(1+p^{1-s})(1-p^{1-2s})}\right), \tag{3.10.7}$$

where the right-hand side defines an analytic function in the open half-plane $\{\mathrm{Re}(s) > \frac{3}{2}\}$ with

$$\begin{aligned}\gamma \;&:=\; \lim_{s\to 3}\frac{\Psi_{D_4^*}(s)}{\Psi^{\mathsf{rot}}_{D_4^*}(s)} = \prod_{p\neq 2}\left(1 - \frac{2(p^2-1)p^{-6}}{(1+p^{-2})(1+p^{-3})(1-p^{-5})}\right) \\ &\approx\; 0.976966019 \;<\; 1.\end{aligned} \tag{3.10.8}$$

Hence, $\sum_{n\leqslant x} c_{D_4^*}(n)$ grows by a factor γ slower than $\sum_{n\leqslant x} c^{\mathsf{rot}}_{D_4^*}(n)$. In particular, we obtain

$$\sum_{n\leqslant x} c_{D_4^*}(n) \;\sim\; \frac{210}{\pi^6}\zeta(3)\gamma\, x^3 \;\approx\; 0.256522\, x^3,$$

as $x \to \infty$. This shows that $\sum_{n\leqslant x} c^{\mathsf{rot}}_{D_4^*}(n)$ and $\sum_{n\leqslant x} c_{D_4^*}(n)$ differ by less than 2.5% asymptotically, which means that it is quite rare that two coincidence rotations that are not symmetry related generate the same CSL.

As we have enumerated the distinct CSLs, we might ask the question of how many non-equivalent CSLs there are, where we call two CSLs Λ_1 and Λ_2 *equivalent* if there is an $R \in \mathrm{O}(\mathbb{J})$ such that $\Lambda_2 = R\Lambda_1$. This question has not completely been answered yet, but some partial results can be found in [93].

3.10.2. The primitive hypercubic lattice $\mathbb{Z}^4$

Let us move on to the primitive hypercubic lattice, which we identify with $\mathbb{Z}^4$ or, in terms of quaternions, with the ring of Lipschitz quaternions $\mathbb{L}$. As $\mathbb{Z}^4$ and D_4^* are commensurate, they have the same group of coincidence rotations, which means

$$\mathrm{SOC}(\mathbb{Z}^4) \;=\; \mathrm{SOC}(D_4^*) \;=\; \mathrm{SO}(4,\mathbb{Q}).$$

Moreover, we have $D_4 \subset \mathbb{Z}^4 \subset D_4^*$, where $\mathbb{Z}^4$ is a sublattice of D_4^* of index 2. Thus, by Theorem 3.7.25, the coincidence indices of the two lattices can differ at most by a factor of 2. This implies that we have either $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$ or $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$ for a given coincidence rotation R. Actually, both cases do occur.

This becomes immediately clear if we recall that the primitive hypercubic lattice $\mathbb{Z}^4$ has a smaller symmetry group than D_4^*. In particular, $\mathrm{SO}(\mathbb{Z}^4)$ contains only 192 rotations, so that

$$[\mathrm{SO}(D_4^*) : \mathrm{SO}(\mathbb{Z}^4)] \;=\; [\mathrm{O}(D_4^*) : \mathrm{O}(\mathbb{Z}^4)] \;=\; 3.$$

As a consequence, every class of symmetry-related coincidence rotations of D_4^* splits into three classes of $\mathbb{Z}^4$. In particular, all rotations in $\mathrm{SO}(D_4^*) \setminus \mathrm{SO}(\mathbb{Z}^4)$ are coincidence rotations for $\mathbb{Z}^4$ of index 2, so we have one class with coincidence index 1 and two classes with index 2.

The same pattern also emerges for the other coincidence rotations — and, more generally, for coincidence isometries as well. In particular, every class of symmetry-related coincidence rotations of D_4^* splits into three classes, one of which has the same coincidence index as before, $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$, while the other two classes have index $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$. To see this, we recall from Theorem 3.7.29 that $\mathrm{den}_{\mathbb{Z}^4}(R)$ divides $\Sigma_{\mathbb{Z}^4}(R)$, while $\Sigma_{\mathbb{Z}^4}(R)$ divides $\mathrm{den}_{\mathbb{Z}^4}(R)^4$. Consequently, $\Sigma_{\mathbb{Z}^4}(R)$ is even if and only if $\mathrm{den}_{\mathbb{Z}^4}(R)$ is. In other words,

$$\Sigma_{\mathbb{Z}^4}(R) \;=\; \mathrm{lcm}\big(\Sigma_{D_4^*}(R), \mathrm{den}_{\mathbb{Z}^4}(R)\big); \tag{3.10.9}$$

compare [4]. If (p, q) is an odd primitive admissible pair, we have

$$\mathrm{den}_{\mathbb{Z}^4}(R(p,q)) \;=\; \begin{cases} |pq|, & \text{if } \langle p|q\rangle \in \mathbb{Z}, \\ 2|pq|, & \text{if } \langle p|q\rangle \notin \mathbb{Z}, \end{cases} \tag{3.10.10}$$

while, if (p, q) is an even primitive admissible pair, one gets

$$\mathrm{den}_{\mathbb{Z}^4}(R(p,q)) \;=\; \begin{cases} \frac{|pq|}{2}, & \text{if } \langle p|q\rangle \text{ is even}, \\ |pq|, & \text{if } \langle p|q\rangle \text{ is odd}. \end{cases} \tag{3.10.11}$$

Checking for all possible combinations of units, we see that every class of symmetry-related coincidence rotations of D_4^* indeed splits into three classes, one of which has odd denominator and coincidence index $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$, while the other two classes have even denominator and coincidence index $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$.

Remark 3.10.12. These relations mean that the coincidence spectrum of $\mathbb{Z}^4$ is larger than the coincidence spectrum of D_4^* and D_4. In particular, we conclude from Remark 3.10.7 that the coincidence spectrum of $\mathbb{Z}^4$ is the set

$$\Sigma\big(\mathrm{OC}(\mathbb{Z}^4)\big) \;=\; \Sigma\big(\mathrm{SOC}(\mathbb{Z}^4)\big) \;=\; (2\mathbb{N}_0{+}1)\cup(4\mathbb{N}_0{+}2). \qquad \Diamond$$

In order to also get an explicit expression for the CSLs, we consider the following chain of inclusions

$$D_4 \cap RD_4 \;\subseteq\; \mathbb{Z}^4 \cap R\mathbb{Z}^4 \;\subseteq\; D_4^* \cap RD_4^* \cap \mathbb{Z}^4 \;\subset\; D_4^* \cap RD_4^* \tag{3.10.12}$$

for any $R \in \mathrm{SOC}(D_4^*)$. As $\Sigma_{D_4}(R) = \Sigma_{D_4^*}(R)$ by Lemma 3.7.4, and also $[D_4^* : D_4] = 4$, we conclude that $[(D_4^* \cap RD_4^*) : (D_4 \cap RD_4)] = 4$. Moreover, with $[D_4^* : \mathbb{Z}^4] = 2$, this shows $[(D_4^* \cap RD_4^* \cap \mathbb{Z}^4) : (D_4 \cap RD_4)] = 2$, as $\Sigma_{D_4^*}(R)$ is always odd. Thus, we are left with two possibilities, namely either with $\mathbb{Z}^4 \cap R\mathbb{Z}^4 = D_4^* \cap RD_4^* \cap \mathbb{Z}^4 = \mathbb{Z}^4 \cap RD_4^*$, in which case $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$, or with $\mathbb{Z}^4 \cap R\mathbb{Z}^4 = D_4 \cap RD_4$, where we have $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$ instead.

Let us summarise these results as follows.

Proposition 3.10.13. *For any coincidence rotation $R \in \mathrm{SOC}(\mathbb{Z}^4)$, the coincidence index is given by*

$$\Sigma_{\mathbb{Z}^4}(R) \;=\; \operatorname{lcm}\bigl(\Sigma_{D_4^*}(R), \operatorname{den}_{\mathbb{Z}^4}(R)\bigr),$$

which is even if and only if $\operatorname{den}_{\mathbb{Z}^4}(R)$ is even. Moreover,

$$\mathbb{Z}^4 \cap R\mathbb{Z}^4 \;=\; \begin{cases} (D_4^* \cap RD_4^*) \cap \mathbb{Z}^4 = \mathbb{Z}^4 \cap RD_4^*, & \text{if } \Sigma_{\mathbb{Z}^4}(R) \text{ is even,} \\ D_4 \cap RD_4, & \text{if } \Sigma_{\mathbb{Z}^4}(R) \text{ is odd,} \end{cases}$$

is the corresponding CSL. □

This allows us to determine the number of coincidence rotations, which is given by $192\, c^{\mathsf{rot}}_{\mathbb{Z}^4}(n)$, as the symmetry group $\mathrm{SO}(\mathbb{Z}^4)$ has order 192. By the above considerations, each class of symmetry-related coincidence rotations splits into three classes, one with coincidence index $\Sigma_{\mathbb{Z}^4}(R) = \Sigma_{D_4^*}(R)$, and two with index $\Sigma_{\mathbb{Z}^4}(R) = 2\Sigma_{D_4^*}(R)$. This gives

$$c^{\mathsf{rot}}_{\mathbb{Z}^4}(n) \;=\; \begin{cases} c^{\mathsf{rot}}_{D_4^*}(n), & \text{if } n \text{ is odd,} \\ 2\, c^{\mathsf{rot}}_{D_4^*}\bigl(\frac{n}{2}\bigr), & \text{if } n \text{ is even.} \end{cases} \tag{3.10.13}$$

As $c^{\mathsf{rot}}_{D_4^*}(n)$ is multiplicative, so is $c^{\mathsf{rot}}_{\mathbb{Z}^4}(n)$, and the corresponding Dirichlet series again admits an Euler product expansion. In particular, we have the following result; compare [4, 93].

Theorem 3.10.14. *The generating function for the number $c^{\mathsf{rot}}_{\mathbb{Z}^4}(n)$ of coincidence rotations of $\mathbb{Z}^4$ is given by*

$$\begin{aligned} \Psi^{\mathsf{rot}}_{\mathbb{Z}^4}(s) \;&=\; \sum_{n=1}^{\infty} \frac{c^{\mathsf{rot}}_{\mathbb{Z}^4}(n)}{n^s} \;=\; (1 + 2^{1-s})\, \Psi^{\mathsf{rot}}_{D_4^*}(s) \\ &=\; \frac{(1 - 2^{1-s})(1 - 2^{2-s})}{1 + 2^{-s}} \, \frac{\zeta(s)\, \zeta(s-1)^2\, \zeta(s-2)}{\zeta(2s)\, \zeta(2s-2)} \\ &=\; (1 + 2^{1-s}) \prod_{p \neq 2} \frac{(1 + p^{-s})(1 + p^{1-s})}{(1 - p^{1-s})(1 - p^{2-s})} \end{aligned}$$

with the first terms being given by

$$\Psi^{\mathsf{rot}}_{\mathbb{Z}^4}(s) = 1 + \frac{2}{2^s} + \frac{16}{3^s} + \frac{36}{5^s} + \frac{32}{6^s} + \frac{64}{7^s} + \frac{168}{9^s} + \frac{72}{10^s} + \frac{144}{11^s} + \frac{196}{13^s} + \frac{128}{14^s} + \frac{576}{15^s} + \frac{324}{17^s} + \frac{336}{18^s} + \frac{400}{19^s} + \frac{1024}{21^s} + \frac{288}{22^s} + \cdots$$

It is a meromorphic function in the complex plane, whose rightmost pole is located at $s = 3$, with residue $\frac{1575}{2\pi^6}\zeta(3)$. Consequently, as $x \to \infty$, we have the asymptotic behaviour

$$\sum_{n \leqslant x} c^{\mathsf{rot}}_{\mathbb{Z}^4}(n) \sim \frac{525}{2\pi^6}\zeta(3)\, x^3 \approx 0.328212\, x^3.$$

Proof. It follows from Eq. (3.10.13) that $\Psi^{\mathsf{rot}}_{\mathbb{Z}^4}(s)$ is obtained from $\Psi^{\mathsf{rot}}_{D_4^*}(s)$ by adding a factor $1+2^{1-s}$. As the latter is analytic, the analytic structure of $\Psi^{\mathsf{rot}}_{\mathbb{Z}^4}(s)$ is the same as that of $\Psi^{\mathsf{rot}}_{D_4^*}(s)$ (see Theorem 3.10.8 and the comments thereafter), except for poles located at $s = 1 + \frac{(2n+1)\pi}{\log(2)}\mathrm{i}$, which are cancelled by the factor $1 + 2^{1-s}$. An application of Theorem 3.4.1 finally yields the asymptotic behaviour. □

In a similar way, we can enumerate the CSLs. It follows from Proposition 3.10.13 that each CSL of D_4^* corresponds to exactly one pair of CSLs of $\mathbb{Z}^4$, one of which has odd index, while the other one has even index. Note that the explicit expressions for the CSLs in Proposition 3.10.13 guarantee that two CSLs of $\mathbb{Z}^4$ are only equal if the corresponding CSLs of D_4^* are equal. This implies that the number of CSLs of $\mathbb{Z}^4$ is given by

$$c_{\mathbb{Z}^4}(n) = \begin{cases} c_{D_4^*}(n), & \text{if } n \text{ is odd,} \\ c_{D_4^*}\left(\frac{n}{2}\right), & \text{if } n \text{ is even.} \end{cases} \tag{3.10.14}$$

This yields the following result.

Theorem 3.10.15. *The generating function for the number $c_{\mathbb{Z}^4}(n)$ of CSLs of $\mathbb{Z}^4$ is given by*

$$\begin{aligned} \Psi_{\mathbb{Z}^4}(s) &= (1+2^{-s})\Psi_{D_4^*}(s) \\ &= (1+2^{-s}) \prod_{p \neq 2} \frac{1 + p^{-s} + 2p^{1-s} + 2p^{-2s} + p^{1-2s} + p^{1-3s}}{(1-p^{2-s})(1-p^{1-2s})} \\ &= 1 + \frac{1}{2^s} + \frac{16}{3^s} + \frac{36}{5^s} + \frac{16}{6^s} + \frac{64}{7^s} + \frac{152}{9^s} + \frac{36}{10^s} + \frac{144}{11^s} + \frac{196}{13^s} \\ &\quad + \frac{64}{14^s} + \frac{576}{15^s} + \frac{324}{17^s} + \frac{152}{18^s} + \frac{400}{19^s} + \frac{1024}{21^s} + \frac{144}{22^s} + \cdots . \end{aligned}$$

It is a meromorphic function in the half-plane $\left\{\mathrm{Re}(s) > \frac{3}{2}\right\}$, whose rightmost pole is located at $s = 3$, with residue $\frac{2835}{4\pi^6}\zeta(3)\gamma$, where γ is the constant from

Eq. (3.10.8). *Consequently, we have the asymptotic behaviour*

$$\sum_{n \leqslant x} c_{\mathbb{Z}^4}(n) \;\sim\; \frac{945}{4\pi^6}\zeta(3)\,\gamma\, x^3 \;\approx\; 0.288587\, x^3,$$

as $x \to \infty$. □

Let us now turn our attention to the corresponding problem of embedded modules, with special focus on the golden ratio.

3.11. More on the icosian ring

The icosian ring, which is a maximal order in the quaternion algebra $\mathbb{H}(\mathbb{Q}(\sqrt{5}))$, is an interesting example of a $\mathbb{Z}$-module of rank 8 that is embedded in $\mathbb{R}^4$. At the same time, it is a $\mathbb{Z}[\tau]$-module of rank 4, and thus an interesting object in our context in its own right. Beyond this, as we already saw in the context of SSLs, it is a powerful tool for the description of the root lattice A_4. Here, we analyse the coincidence structure, first via the CSLs for A_4 and then via the CSMs for $\mathbb{I}$ itself.

3.11.1. Coincidences of the root lattice A_4

Recall from Section 3.5.4 that A_4 can be represented as

$$L \;=\; \{x \in \mathbb{I} \mid x = \widetilde{x}\},$$

which brings in the icosian ring, $\mathbb{I}$. As $\mathbb{J}$ and $\mathbb{I}$ share a lot of properties, we expect the calculation of the CSLs to be similar. Indeed, this is true, and we may thus skip various details; see [16, 55, 97] for details. However, recall that we needed a pair of quaternions to characterise the CSLs of $\mathbb{J}$. Here, we only need a *single* quaternion q, as the coincidence rotations of A_4 can be parametrised by admissible pairs of the form $(q, \widetilde{q})$. Consequently, we call a quaternion $q \in \mathbb{I}$ *admissible*, if $|q\widetilde{q}|^2 = \mathrm{nr}(|q|^2)$ is a square in $\mathbb{N}$. In fact, $x \mapsto \frac{1}{|q\widetilde{q}|} qx\widetilde{q}$ defines a coincidence rotation of A_4 in the above representation if and only if $q \in \mathbb{I}$ is admissible.

In the case of the hypercubic lattices in four dimensions, it was useful to deal with an extended admissible pair of primitive quaternions. Here, we define the notion of an extended primitive admissible quaternion as follows. Let $q \in \mathbb{I}$ be primitive and admissible. Then, $\frac{|q\widetilde{q}|^2}{\gcd(|q|^2, |\widetilde{q}|^2)^2}$ is a square in $\mathbb{Z}[\tau]$. Here, gcd refers to the greatest common divisor in $\mathbb{Z}[\tau]$, which is well defined up to a unit as $\mathbb{Z}[\tau]$ is a Euclidean domain. Now, $\frac{|q|^2}{\gcd(|q|^2, |\widetilde{q}|^2)} \in \mathbb{Z}[\tau]$ and $\frac{|\widetilde{q}|^2}{\gcd(|q|^2, |\widetilde{q}|^2)} \in \mathbb{Z}[\tau]$ are relatively prime in $\mathbb{Z}[\tau]$. Since their product is a square, they must be squares (up to units) in $\mathbb{Z}[\tau]$, too (we have unique prime factorisation). If the units have been chosen appropriately, we may assume

that $\frac{|q|^2}{\gcd(|q|^2,|\widetilde{q}|^2)} \in \mathbb{Z}[\tau]$ and $\frac{|\widetilde{q}|^2}{\gcd(|q|^2,|\widetilde{q}|^2)} \in \mathbb{Z}[\tau]$ are squares in $\mathbb{Z}[\tau]$. Hence, we may take the root (where we may choose the positive one) and define

$$\alpha_q := \sqrt{\frac{|\widetilde{q}|^2}{\gcd(|q|^2,|\widetilde{q}|^2)}}, \quad \alpha_{\widetilde{q}} := \alpha_q' = \sqrt{\frac{|q|^2}{\gcd(|q|^2,|\widetilde{q}|^2)}}, \tag{3.11.1}$$

which are unique up to units. Note further that the last equality only holds up to a unit.

Definition 3.11.1. Let $q \in \mathbb{I}$ be a primitive admissible quaternion. Then, $q_\alpha := \alpha_q q$ is called an *extended admissible quaternion* (corresponding to q).

Of course, this definition is unique only up to units in $\mathbb{Z}[\tau]$, but this does not matter as units of $\mathbb{Z}[\tau]$ cancel out in the definition of the coincidence rotations. The key result in the determination of the CSLs is the following characterisation.

Theorem 3.11.2 ([16, Thms. 2 and 3])**.** *Let $q \in \mathbb{I}$ be a primitive admissible quaternion and q_α its extension. Then,*

$$L \cap \frac{qL\widetilde{q}}{|q\widetilde{q}|} \;=\; L_{q_\alpha} \;:=\; (q_\alpha \mathbb{I} + \mathbb{I}\widetilde{q}_\alpha) \cap L.$$

Moreover, its coincidence index $\Sigma_{A_4}(q)$ is given by

$$\Sigma_{A_4}(q) \;=\; |q_\alpha|^2 \;=\; \operatorname{lcm}\bigl(|q|^2, |\widetilde{q}|^2\bigr). \qquad \square$$

This allows us to determine the multiplicative counting function $c_{A_4}^{\mathsf{rot}}$, which is given by [97, Eq. (5.29)]

$$c_{A_4}^{\mathsf{rot}}(p^r) \;=\; \begin{cases} 6 \cdot 5^{2r-1}, & \text{if } p = 5, \\ \frac{p+1}{p-1} p^{r-1}(p^{r+1} + p^{r-1} - 2), & \text{if } p \equiv \pm 1 \ (5), \\ p^{2r} + p^{2r-2}, & \text{if } p \equiv \pm 2 \ (5). \end{cases} \tag{3.11.2}$$

The result now reads as follows.

Theorem 3.11.3 ([16, Thm. 4])**.** *Let $120\, c_{A_4}^{\mathsf{rot}}(m)$ be the number of coincidence rotations of index m of the root lattice A_4, as specified by Eq.* (3.11.2)*. Then, with $K = \mathbb{Q}(\sqrt{5}\,)$, the Dirichlet series generating function for $c_{A_4}^{\mathsf{rot}}(m)$ reads*

$$\begin{aligned} \Psi_{A_4}^{\mathsf{rot}}(s) \;&=\; \sum_{n \in \mathbb{N}} \frac{c_{A_4}^{\mathsf{rot}}(n)}{n^s} \;=\; \frac{\zeta_K(s-1)}{1+5^{-s}} \frac{\zeta(s)\zeta(s-2)}{\zeta(2s)\zeta(2s-2)} \\ &=\; \frac{1+5^{1-s}}{1-5^{2-s}} \prod_{p \equiv \pm 1 (5)} \frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})} \prod_{p \equiv \pm 2 (5)} \frac{1+p^{-s}}{1-p^{2-s}} \\ &=\; 1 + \tfrac{5}{2^s} + \tfrac{10}{3^s} + \tfrac{20}{4^s} + \tfrac{30}{5^s} + \tfrac{50}{6^s} + \tfrac{50}{7^s} + \tfrac{80}{8^s} + \tfrac{90}{9^s} + \tfrac{150}{10^s} + \tfrac{144}{11^s} + \cdots, \end{aligned}$$

and the coincidence spectrum is $\mathbb{N}$. □

The function $\Psi_{A_4}^{\mathsf{rot}}$ is meromorphic in the entire complex plane, and its rightmost pole is a simple pole at $s = 3$, with residue

$$\begin{aligned} \rho_{A_4}^{\mathsf{rot}} &= \operatorname{res}_{s=3}\bigl(\Psi_{A_4}^{\mathsf{rot}}(s)\bigr) = \frac{125}{126}\,\frac{\zeta_K(2)\zeta(3)}{\zeta(6)\zeta(4)} \\ &= \frac{450\sqrt{5}}{\pi^6}\,\zeta(3) \approx 1.258124, \end{aligned} \tag{3.11.3}$$

where the last equation follows by inserting the special values

$$\zeta(4) = \frac{\pi^4}{90}, \quad \zeta(6) = \frac{\pi^6}{945}, \quad \zeta_K(2) = \frac{2\pi^4}{75\sqrt{5}}, \quad L(1,\chi_5) = \frac{2\log(\tau)}{\sqrt{5}},$$

and Apéry's constant $\zeta(3) \approx 1.202056903$; see [11, 16] and references therein.

A familiar argument based on Theorem 3.4.1 gives us the asymptotic growth rate of $c_{A_4}^{\mathsf{rot}}(m)$ as follows.

Corollary 3.11.4. *With the residue* $\rho_{A_4}^{\mathsf{rot}}$ *from Eq.* (3.11.3)*, the summatory asymptotic behaviour of* $c_{A_4}^{\mathsf{rot}}(m)$ *is given by*

$$\sum_{m \leqslant x} c_{A_4}^{\mathsf{rot}}(m) \sim \rho_{A_4}^{\mathsf{rot}}\,\frac{x^3}{3} \approx 0.419375\,x^3,$$

as $x \to \infty$. □

As we shall see later in Corollary 3.11.7, the number of coincidence rotations and the number of CSLs of a given index grow much faster than the number of SSLs. This is due to the fact that the index of a primitive SSL is $\operatorname{den}_{A_4}(q)^4$, whereas the coincidence index $\Sigma_{A_4}(q)$ is much smaller and satisfies the inequality $\operatorname{den}_{A_4}(q) \leqslant \Sigma_{A_4}(q) \leqslant \bigl(\operatorname{den}_{A_4}(q)\bigr)^2$.

The key result in counting the number of distinct CSLs is the following.

Theorem 3.11.5 ([55, Thm. 7])**.** *Assume that* q_1 *and* q_2 *are admissible. Then, one has* $L(R(q_1)) = L(R(q_2))$ *if and only if* $|q_1|^2 = |q_2|^2$ *and* $\operatorname{gcld}(q_1, |q_1\widetilde{q}_1|/c) = \operatorname{gcld}(q_2, |q_2\widetilde{q}_2|/c)$*, where* $c = \sqrt{5}$ *if* $|q_1|^2 = |q_2|^2$ *is divisible by* 5*, and* $c = 1$ *otherwise.* □

From this result, one can derive the following expression for the counting function [97, Eq. (5.93)]

$$c_{A_4}(p^r) = \begin{cases} 6 \cdot 5^{2r-2}, & \text{if } p = 5, \\ \frac{(p+1)^2}{p^3-1}\bigl(p^{2r+1} + p^{2r-2} - 2p^{\frac{r-1}{2}}\bigr), & \text{if } p \equiv \pm 1 \ (5),\ r \text{ odd}, \\ \frac{(p+1)^2}{p^3-1}\bigl(p^{2r+1} + p^{2r-2} - 2\frac{p^2+1}{p+1}p^{\frac{r-2}{2}}\bigr), & \text{if } p \equiv \pm 1 \ (5),\ r \text{ even}, \\ p^{2r} + p^{2r-2}, & \text{if } p \equiv \pm 2 \ (5). \end{cases}$$

We can now summarise as follows.

Theorem 3.11.6 ([97, Thm. 5.5.6])**.** *Let $c_{A_4}(m)$ be the number of CSLs of the root lattice A_4 of index m. The Dirichlet series generating function for $c_{A_4}(m)$ reads*

$$\begin{aligned}\Psi_{A_4}(s) \,=\, \sum_{n\in\mathbb{N}} \frac{c_{A_4}(n)}{n^s} \,&=\, \Big(1+\frac{6\cdot 5^{-s}}{1-5^{2-s}}\Big) \prod_{p\equiv\pm 2(5)} \frac{1+p^{-s}}{1-p^{2-s}} \\ &\quad\times \prod_{p\equiv\pm 1(5)} \frac{1+p^{-s}+2p^{1-s}+2p^{-2s}+p^{1-2s}+p^{1-3s}}{(1-p^{2-s})(1-p^{1-2s})} \\ &= 1+\tfrac{5}{2^s}+\tfrac{10}{3^s}+\tfrac{20}{4^s}+\tfrac{6}{5^s}+\tfrac{50}{6^s}+\tfrac{50}{7^s}+\tfrac{80}{8^s}+\tfrac{90}{9^s}+\tfrac{30}{10^s}+\tfrac{144}{11^s}+\cdots . \qquad \square\end{aligned}$$

In order to compare $\Psi_{A_4}(s)$ and $\Psi_{A_4}^{\mathsf{rot}}(s)$, we consider the function

$$\begin{aligned}\psi_{A_4}(s) \,&:=\, \frac{\Psi_{A_4}(s)}{\Psi_{A_4}^{\mathsf{rot}}(s)} \\ &=\, \Big(1-\frac{24\cdot 5^{-s}}{1+5^{1-s}}\Big) \prod_{p\equiv\pm 1(5)} \Big(1-\frac{2(p^2-1)p^{-2s}}{(1+p^{-s})(1+p^{1-s})(1-p^{1-2s})}\Big).\end{aligned}$$

It is analytic in the open half-plane $\{\mathrm{Re}(s) > \frac{3}{2}\}$, as the Euler product converges there. This proves that $\Psi_{A_4}(s)$ is a meromorphic function in the open half-plane $\{\mathrm{Re}(s) > \frac{3}{2}\}$. Its rightmost pole is a simple pole at $s = 3$ with residue

$$\rho_{A_4} \,=\, \mathrm{res}_{s=3}\big(\Psi_{A_4}(s)\big) \,=\, \psi_{A_4}(3)\,\rho_{A_4}^{\mathsf{rot}} \,\approx\, 1.025695, \tag{3.11.4}$$

where $\psi_{A_4}(3) \approx 0.815257622 < 1$ has been calculated numerically. Finally, we apply Theorem 3.4.1, which gives us the asymptotic growth rate as follows.

Corollary 3.11.7. *With the residue ρ_{A_4} from Eq.* (3.11.4)*, the summatory asymptotic behaviour of $c_{A_4}(m)$ is given by*

$$\sum_{m\leqslant x} c_{A_4}(m) \,\sim\, \rho_{A_4}\frac{x^3}{3} \,\approx\, 0.341898\, x^3,$$

as $x \to \infty$. $\square$

Comparing the growth rate of the number of CSLs with that of the coincidence rotations, we see that the former is roughly 20% lower than the latter. As we shall see shortly, this difference is much bigger than in the case of the icosian ring. Yet, it is still more an exception than a rule that two coincidence rotations that are not symmetry related generate the same CSL.

3.11.2. Coincidences of $\mathbb{I}$

Here, we want to consider the CSMs of the icosian ring $\mathbb{I}$ itself, which is an interesting example of an embedded module in 4-space. It is also a $\mathbb{Z}[\tau]$-lattice in $\mathbb{R}^4$ in the sense of Definition 3.6.2.

The methods to find the CSMs are basically a combination of the tools we used in Sections 3.10 and 3.11.1, as we deal with admissible pairs of quaternions in $\mathbb{I}$ here. Thus, we will keep the presentation concise and refer to [97] for details.

As $\mathbb{I}$ is a $\mathbb{Z}(\tau)$-lattice, we have $\mathrm{scal}_{\mathbb{I}}(\mathbb{1}) = \mathbb{Q}(\tau)^{\times}$ and $\mathrm{Scal}_{\mathbb{I}}(\mathbb{1}) = \mathbb{Z}(\tau)$. Correspondingly, we call a pair $(p, q) \in \mathbb{I}\times\mathbb{I}$ *primitive admissible* if p, q are primitive and $|pq|^2$ is a square in $\mathbb{Z}[\tau]$. It follows that the coincidence rotations are precisely those rotations $R(q, p)x = qxp/|pq|$ that can be parametrised by a primitive admissible pair; compare [97].

As before, it makes sense to define

$$\alpha_q \,:=\, \sqrt{\frac{|p|^2}{\gcd(|q|^2, |p|^2)}} \quad\text{and}\quad \alpha_p \,:=\, \sqrt{\frac{|q|^2}{\gcd(|q|^2, |p|^2)}} \tag{3.11.5}$$

for any primitive admissible pair (q, p), where α_q and α_p are again defined up to a unit (now in $\mathbb{Z}[\tau]$). Correspondingly, we call $(q_\alpha, p_\alpha) = (\alpha_q q, \alpha_p p)$ the extension of the primitive admissible pair (q, p). This implies

$$|q_\alpha|^2 \,=\, |p_\alpha|^2 \,=\, |q_\alpha p_\alpha| \quad \text{(up to a unit)}. \tag{3.11.6}$$

The CSMs of $\mathbb{I}$ can now completely be characterised as follows, which is the analogue of Theorem 3.10.4 for the Hurwitz ring $\mathbb{J}$.

Theorem 3.11.8 ([97, Thm. 5.4.2 and 5.4.4])**.** *Let (q_α, p_α) be the extension of the primitive admissible pair (q, p). Then, one has*

$$\mathbb{I} \cap \frac{q\mathbb{I}p}{|qp|} \,=\, q_\alpha\mathbb{I} + \mathbb{I}p_\alpha\,.$$

The index of this CSM in $\mathbb{I}$ is given by

$$\Sigma_{\mathbb{I}}\big(R(q,p)\big) \,=\, \mathrm{nr}\big(\mathrm{lcm}(|q|^2, |p|^2)\big) \,=\, \mathrm{nr}\big(|q_\alpha|^2\big) \,=\, \mathrm{nr}\big(|p_\alpha|^2\big). \qquad \square$$

This allows us to calculate the number of coincidence rotations of a given index m, which is given by $7200\, c_{\mathbb{I}}^{\mathsf{rot}}(m)$, where the factor 7200 is the order of $\mathrm{SO}(\mathbb{I})$, the rotation symmetry group of $\mathbb{I}$, and $c_{\mathbb{I}}^{\mathsf{rot}}(m)$ is a multiplicative function which is completely determined by

$$c_{\mathbb{I}}^{\mathsf{rot}}(p^r) \,=\, \begin{cases} 3\cdot 5^{r-1}(13\cdot 5^{r-1} - 1), & \text{if } p = 5, r \geqslant 1,\\ h(p, r), & \text{if } p \equiv \pm 1 \ (5) \text{ and } r \geqslant 1,\\ \frac{p^2+1}{p^2-1}\, p^{2r-2}(p^{2r+2} + p^{2r-2} - 2), & \text{if } p \equiv \pm 2 \ (5) \text{ and } r \geqslant 2 \text{ even},\\ 0, & \text{if } p \equiv \pm 2 \ (5) \text{ and } r \geqslant 1 \text{ odd}, \end{cases}$$

with

$$\begin{aligned} h(p,r) \;=\; & 2p^{2r-2}(p+1)^2 - 4p^{r-2}\frac{p^{r-1}-1}{(p-1)^3}(3p^2+1)(p+1) \\ & + (r-1)\frac{(p+1)^2}{(p-1)^2}p^{r-2}\big(p^{r-2}(p^2+1)^2+4\big). \end{aligned} \tag{3.11.7}$$

Thus, we can calculate the corresponding generating function.

Theorem 3.11.9 ([97, Thm. 5.4.5])**.** *Let* $7200\,c_{\mathbb{I}}^{\mathsf{rot}}(m)$ *be the number of coincidence rotations of the icosian ring* $\mathbb{I}$*. Then, the Dirichlet series generating function for* $c_{\mathbb{I}}^{\mathsf{rot}}(m)$ *reads*

$$\begin{aligned} \Psi_{\mathbb{I}}^{\mathsf{rot}}(s) \;&=\; \sum_{n\in\mathbb{N}} \frac{c_{\mathbb{I}}^{\mathsf{rot}}(n)}{n^s} \;=\; \zeta_{\mathbb{I}}^{\mathsf{pr}}(s)\,\zeta_{\mathbb{I}}^{\mathsf{pr}}(s-1) \\ &=\; \frac{(1+5^{-s})(1+5^{1-s})}{(1-5^{1-s})(1-5^{2-s})} \\ &\quad\times \prod_{p\equiv\pm1(5)} \left(\frac{(1+p^{-s})(1+p^{1-s})}{(1-p^{1-s})(1-p^{2-s})}\right)^2 \prod_{p\equiv\pm2(5)} \frac{(1+p^{-2s})(1+p^{2-2s})}{(1-p^{2-2s})(1-p^{4-2s})} \\ &=\; 1+\tfrac{25}{4^s}+\tfrac{36}{5^s}+\tfrac{100}{9^s}+\tfrac{288}{11^s}+\tfrac{440}{16^s}+\tfrac{400}{19^s}+\tfrac{900}{20^s}+\tfrac{960}{25^s}+\tfrac{1800}{29^s}+\cdots \end{aligned}$$

with $\zeta_{\mathbb{I}}^{\mathsf{pr}}(s)$ *as given in Eq.* (3.5.18)*. In particular, the possible coincidence indices are exactly those numbers that can be represented by the quadratic form* $k^2+k\ell-\ell^2 = \mathrm{nr}(k+\ell\tau)$*.* □

$\Psi_{\mathbb{I}}^{\mathsf{rot}}(s)$ is a meromorphic function in the entire complex plane, whose rightmost pole is a simple pole at $s=3$ with residue (see [97, Eq. (5.61)])

$$\begin{aligned} \rho_{\mathbb{I}}^{\mathsf{rot}} \;&:=\; \mathrm{res}_{s=3}\big(\Psi_{\mathbb{I}}^{\mathsf{rot}}(s)\big) \;=\; \frac{\zeta_K(2)^2\zeta_K(3)}{\zeta_K(4)\zeta_K(6)}L(1,\chi_5) \\ &=\; \frac{3^5\,5^7\,7\sqrt{5}}{268\pi^{12}}\log(\tau)\zeta_K(3) \;\approx\; 0.593177. \end{aligned} \tag{3.11.8}$$

Using Theorem 3.4.1, we get the following asymptotic behaviour.

Corollary 3.11.10 ([97, Cor. 5.4.6])**.** *The asymptotic behaviour of the summatory function of* $c_{\mathbb{I}}^{\mathsf{rot}}(m)$*, as* $x\to\infty$*, is*

$$\sum_{m\leqslant x} c_{\mathbb{I}}^{\mathsf{rot}}(m) \;\sim\; \rho_{\mathbb{I}}^{\mathsf{rot}}\frac{x^3}{3} \;\approx\; 0.197726\,x^3,$$

with $\rho_{\mathbb{I}}^{\mathsf{rot}}$ *as given in Eq.* (3.11.8)*.* □

In order to enumerate the CSMs themselves, we need a criterion that tells us which rotations generate the same CSM. This is given by the following result, which is the analogue of Theorem 3.10.9 for $\mathbb{J}$, and of Theorem 3.11.5 for the lattice A_4.

Theorem 3.11.11 ([97, Thm. 5.4.13]). *Let (q_1, p_1) and (q_2, p_2) be two primitive admissible pairs. Then,*

$$\mathbb{I} \cap \frac{q_1 \mathbb{I} p_1}{|q_1 p_1|} = \mathbb{I} \cap \frac{q_2 \mathbb{I} p_2}{|q_2 p_2|}$$

holds if and only if the following conditions are satisfied (up to units).

(1) $|q_1 p_1| = |q_2 p_2|$,
(2) $\operatorname{lcm}(|q_1|^2, |p_1|^2) = \operatorname{lcm}(|q_2|^2, |p_2|^2)$,
(3) $\operatorname{gcld}(q_1, |p_1 q_1|) = \operatorname{gcld}(q_2, |p_2 q_2|)$, *and*
(4) $\operatorname{gcrd}(p_1, |p_1 q_1| = \operatorname{gcrd}(p_2, |p_2 q_2|)$. □

The effect of these criteria is that it is now a purely combinatorial task to calculate $c_{\mathbb{I}}(m)$ and the corresponding Dirichlet series. For explicit expressions for $c_{\mathbb{I}}(m)$, see [97, Eq. 5.79].

Theorem 3.11.12 ([97, Thm. 5.4.14]). *Let $c_{\mathbb{I}}(m)$ be the number of CSMs of the icosian ring $\mathbb{I}$ of index m. Then, the Dirichlet series generating function for $c_{\mathbb{I}}(m)$ reads*

$$\begin{aligned}\Psi_{\mathbb{I}}(s) = \sum_{n\in\mathbb{N}} \frac{c_{\mathbb{I}}(n)}{n^s} &= \frac{1 + 11\cdot 5^{-s} + 7\cdot 5^{-2s} + 5^{1-3s}}{(1-5^{2-s})(1-5^{1-2s})} \\ &\quad \times \prod_{p\equiv\pm 1(5)} \left(\frac{1 + p^{-s} + 2p^{1-s} + 2p^{-2s} + p^{1-2s} + p^{1-3s}}{(1-p^{2-s})(1-p^{1-2s})}\right)^2 \\ &\quad \times \prod_{p\equiv\pm 2(5)} \frac{1 + p^{-2s} + 2p^{2-2s} + 2p^{-4s} + p^{2-4s} + p^{2-6s}}{(1-p^{4-2s})(1-p^{2-4s})} \\ &= 1 + \tfrac{25}{4^s} + \tfrac{36}{5^s} + \tfrac{100}{9^s} + \tfrac{288}{11^s} + \tfrac{410}{16^s} + \tfrac{400}{19^s} + \tfrac{900}{20^s} + \tfrac{912}{25^s} + \tfrac{1800}{29^s} + \cdots . \quad \square\end{aligned}$$

We are not aware of a representation of $\Psi_{\mathbb{I}}(s)$ in terms of zeta functions. Nevertheless, we can determine its analytic properties. We note that the Euler product

$$\begin{aligned}\psi_{\mathbb{I}}(s) := \frac{\Psi_{\mathbb{I}}(s)}{\Psi_{\mathbb{I}}^{\mathsf{rot}}(s)} &= \left(1 - \frac{48\cdot 5^{-2s}}{(1+5^{-s})(1+5^{1-s})(1-5^{1-2s})}\right) \\ &\quad \times \prod_{p\equiv\pm 1(5)} \left(1 - \frac{2(p^2-1)p^{-2s}}{(1+p^{-s})(1+p^{1-s})(1-p^{1-2s})}\right)^2 \\ &\quad \times \prod_{p\equiv\pm 2(5)} \left(1 - \frac{2(p^4-1)p^{-4s}}{(1+p^{-2s})(1+p^{2-2s})(1-p^{2-4s})}\right)\end{aligned} \tag{3.11.9}$$

converges for $\operatorname{Re}(s) > \frac{3}{2}$, which implies that $\Psi_{\mathbb{I}}(s)$ is meromorphic in the half-plane $\left\{\operatorname{Re}(s) > \frac{3}{2}\right\}$. Moreover, the rightmost pole of $\Psi_{\mathbb{I}}(s)$ is a simple

pole located at $s = 3$, with residue

$$\rho_{\mathbb{I}} := \operatorname{res}_{s=3}\big(\Psi_{\mathbb{I}}(s)\big) = \psi_{\mathbb{I}}(3)\rho_{\mathbb{I}}^{\mathsf{rot}} \approx 0.587063. \tag{3.11.10}$$

Here, $\psi_{\mathbb{I}}(3) \approx 0.989691798 < 1$ was calculated numerically. Finally, we apply Theorem 3.4.1 to obtain the asymptotic behaviour.

Corollary 3.11.13 ([97, Cor. 5.4.15])**.** *The asymptotic behaviour of the summatory function of $c_{\mathbb{I}}(m)$, as $x \to \infty$, is*

$$\sum_{m \leqslant x} c_{\mathbb{I}}(m) \sim \rho_{\mathbb{I}} \frac{x^3}{3} \approx 0.195688\, x^3, \tag{3.11.11}$$

with $\rho_{\mathbb{I}}$ as given above. □

Note that $\rho_{\mathbb{I}}$ and $\rho_{\mathbb{I}}^{\mathsf{rot}}$ differ by just about 1%. Thus, in most cases, two coincidence rotations that are not symmetry related generate different CSMs.

3.12. Multiple CSLs of the cubic lattices

So far, we have mostly considered ordinary (or simple) CSLs and CSMs. The problem of finding all *multiple* CSLs (MCSLs) is more difficult than determining all CSLs. In fact, there are only few cases where the problem of multiple coincidences has been solved so far. These include the two-dimensional lattices and modules of n-fold symmetry [4], which we discussed in Section 3.8, and the three-dimensional cubic lattices, which we want to discuss here; compare [94, 97].

Let us recall from Section 3.9 that any coincidence rotation R of the cubic lattices can be parametrised by primitive Hurwitz quaternions. Moreover, there is a bijection between the CSLs of the body-centred cubic lattice and the ideals $q\mathbb{J}$ generated by odd primitive quaternions. In particular, we have $\Gamma_{\mathsf{bcc}} = \mathrm{Im}(\mathbb{J})$ and $\Gamma_{\mathsf{bcc}}(R(q)) = \mathrm{Im}(q\mathbb{J})$ with $\Sigma(R(q)) = |q|^2$ if q is a primitive odd quaternion. If q is an even primitive quaternion, then $\Sigma(R(q)) = \frac{|q|^2}{2}$. In this case, q can be written as the product $r\,(1,1,0,0)$ of an odd primitive quaternion with an even one, and the corresponding CSL can be written as $\Gamma_{\mathsf{bcc}}(R(q)) = \mathrm{Im}(r\mathbb{J})$.

Consequently, it is sufficient to consider CSLs generated by primitive odd quaternions. Just as in the case of ordinary CSLs, we start with the analysis of the body-centred cubic lattice and later derive the MCSLs of the other cubic lattices in the setting of Eq. (3.9.1).

Let us first discuss the coincidence spectrum. We know from Remark 3.9.6 that the ordinary coincidence spectrum for all three types of cubic lattices is $2\mathbb{N}_0 + 1$. Moreover, we have seen in Section 3.7.2 that $\Sigma(R_1, \ldots, R_m)$ divides the product $\Sigma(R_1) \cdot \ldots \cdot \Sigma(R_m)$. Thus, the spectrum of indices of MCSLs is again the set of positive odd integers.

Proposition 3.12.1. *Let Γ be any cubic lattice. The (multiple) coincidence spectrum of Γ is $2\mathbb{N}_0 + 1$.* □

Hence, no new indices occur. Nevertheless, additional lattices emerge and the multiplicity of the corresponding index will increase. We have seen that $c_\Gamma(m)$ is a multiplicative function. By Theorem 3.7.19, this implies that any ordinary CSL can be written as $\Gamma(R) = \Gamma(R_1) \cap \ldots \cap \Gamma(R_n)$, where the indices $\Sigma_\Gamma(R_i)$ are powers of distinct primes. In this case, the MCSL $\Gamma(R_1) \cap \ldots \cap \Gamma(R_n)$ agrees with an ordinary CSL. However, if the indices of the $\Gamma(R_i)$ are not relatively prime, the corresponding MCSL is, in general, not equal to an ordinary CSL.

More generally, by an application of Theorem 3.7.19, the multiplicativity of $c_\Gamma(m)$ guarantees that *any* MCSL $\Gamma(R_1, \ldots, R_n)$ can be written as the intersection of MCSLs Γ_k of prime power index. Furthermore, the Γ_k can be chosen in such a way that they are intersections of at most n ordinary CSLs. Thus, we may restrict our analysis of MCSLs to those MCSLs whose index is a prime power.

To become more concrete, we mention that the decomposition of CSLs into CSLs of prime power index corresponds to the prime factorisation in $\mathbb{J}$. In particular, if $|q|^2 = \pi_1^{\alpha_1} \cdot \ldots \cdot \pi_k^{\alpha_k}$ is the prime factorisation of $|q|^2$ in $\mathbb{N}$ and $p_i := \gcld(q, \pi_i^{\alpha_i})$, the aforementioned decomposition is now given by $\Gamma(R(q)) = \Gamma(R(p_1)) \cap \ldots \cap \Gamma(R(p_k))$. Note that q is a common right multiple of all p_i. Conversely, if the p_i are primitive odd quaternions such that all $|p_i|^2$ are relatively prime, then any least common right multiple q is primitive and odd, and we have $\Gamma(R(q)) = \Gamma(R(p_1)) \cap \ldots \cap \Gamma(R(p_k))$. Likewise, if we define $p_{ij} = \gcld(q_i, \pi_j^{\alpha_{ij}})$, where the α_{ij} are the exponents in the prime factorisation $|q_i|^2 = \pi_1^{\alpha_{i1}} \cdot \ldots \cdot \pi_k^{\alpha_{ik}}$, then the corresponding decomposition of the MCSL reads $\Gamma(R(q_1), \ldots, R(q_n)) = \Gamma_1 \cap \ldots \cap \Gamma_k$ with $\Gamma_\ell = \Gamma(R(p_{1\ell})) \cap \ldots \cap \Gamma(R(p_{n\ell}))$.

Moreover, this guarantees the multiplicativity of the corresponding counting functions $c^{(\infty)}(m)$ and $c^{(k)}(m)$, where $c^{(\infty)}(m)$ is the number of all MCSLs of a given index m and $c^{(k)}(m)$ the corresponding number of all MCSLs that can be written as the intersection of at most k ordinary CSLs.

As we want to enumerate the distinct MCSLs, it is an essential question under what condition two MCSLs are equal. A preliminary result is the following, which generalises Lemma 3.7.33 to the present situation.

Lemma 3.12.2 ([97, Lemma 6.1.2])**.** *Let Γ be any cubic lattice and assume that*

$$\Gamma\big(R(q_1), \ldots, R(q_n)\big) \;=\; \Gamma\big(R(q_1'), \ldots, R(q_m')\big),$$

where q_i and q_j' are primitive odd quaternions. Then, we have

$$\Sigma_\Gamma\big(R(q_1), \ldots, R(q_n)\big) \;=\; \Sigma_\Gamma\big(R(q_1'), \ldots, R(q_m')\big)$$

together with $\operatorname{lcm}\left(|q_1|^2,\dots,|q_n|^2\right) = \operatorname{lcm}\left(|q'_1|^2,\dots,|q'_n|^2\right)$. □

The conditions of the lemma are necessary, but by no means sufficient. For ordinary CSLs, we have the much stronger condition $q\mathbb{J} = q'\mathbb{J}$, and we expect additional conditions for MCSLs. Let us start with the case $n = 2$.

3.12.1. Intersections of two CSLs

As the body-centred cubic lattice $\Gamma = \Gamma_{\mathsf{bcc}} = \operatorname{Im}(\mathbb{J})$ has the most convenient representation in terms of quaternions, we start with this lattice. The first step to determine all possible MCSLs $\Gamma(R_1, R_2)$ that can be written as the intersection of at most two ordinary CSLs is the calculation of their indices. We note that $\Gamma_+(R_1, R_2) := \Gamma(R_1)+\Gamma(R_2) = \operatorname{Im}(q_1\mathbb{J}+q_2\mathbb{J}) = \operatorname{Im}(q\mathbb{J})$, where $q = \operatorname{gcld}(q_1, q_2)$. Hence, recalling that we may assume $|q_i|^2$ to be odd, we have

$$\Sigma(R_1, R_2) \;=\; \frac{|q_1|^2|q_2|^2}{|q|^2}. \tag{3.12.1}$$

In the case that $|q_1|^2$ and $|q_2|^2$ are relatively prime, this reduces to the relation $\Sigma(R_1, R_2) = |q_1|^2|q_2|^2$. This is the aforementioned case where the MCSL is equal to an ordinary CSL. Another special case occurs when q_1 is a left divisor of q_2. Here, we have $\Gamma(R_2) \subseteq \Gamma(R_1)$, and the MCSL $\Gamma(R_1, R_2) = \Gamma(R_2)$ is again an ordinary CSL. In order to understand the general situation, we start with the case that both $|q_i|^2$ are powers of the same rational prime p.

Actually, the case of MCSLs of prime power index is sufficient, because we can recover the general case from this one, as we have mentioned before. We are mainly interested in the case of two different CSLs none of which is a sublattice of the other one, so neither q_1 nor q_2 is a right multiple of the other one. Fortunately, we do not need to exclude the latter case explicitly, as all formulas include the case of ordinary CSLs implicitly.

Recall that we have an explicit expression for ordinary CSLs, namely $\Gamma_{\mathsf{bcc}}(R(q)) = \operatorname{Im}(q\mathbb{J})$. An analogous expression for MCSLs is given by the following result.

Lemma 3.12.3 ([97, Lemma 6.2.2])**.** *Let q_1 and q_2 be primitive quaternions with $|q_i|^2 = p^{\alpha_i}$, where p is the same odd prime for both quaternions. Let q be a least common right multiple of q_1 and q_2. Then, we have*

$$\Gamma_{\mathsf{bcc}}(R_1, R_2) \;=\; \operatorname{Im}(q\mathbb{J}+q_1\mathbb{J}\bar{q}_2) \;=\; \operatorname{Im}(q\mathbb{J}+q_2\mathbb{J}\bar{q}_1).$$ □

Note that $q\mathbb{J} + q_1\mathbb{J}\bar{q}_2$ need not be an ideal. If not, $\Gamma_{\mathsf{bcc}}(R_1, R_2)$ is neither an ordinary CSL nor a multiple of one. Further, note that $\operatorname{Im}(q\mathbb{J})$ is a multiple of an ordinary CSL as q, in general, is not primitive here.

When enumerating MCSLs, we must make sure that we do not count any MCSL twice. Thus, we need a criterion when two MCSLs are equal. This is provided by the following result.

Theorem 3.12.4 ([97, Thm. 6.2.3])**.** *Let q_i with $1 \leqslant i \leqslant 4$ be primitive quaternions such that $|q_i|^2 = p^{\alpha_i}$, where p is an odd rational prime and where $\alpha_1 \geqslant \alpha_2 \geqslant \alpha_4$ and $\alpha_3 \geqslant \alpha_4$. Let q_{ij} with $|q_{ij}|^2 = p^{\alpha_{ij}}$ be the greatest common left divisor of q_i and q_j. In addition, if $\alpha_1 = \alpha_2$, let $\alpha_{13} \geqslant \alpha_{23}$, and if $\alpha_3 = \alpha_4$, let $\alpha_{13} \geqslant \alpha_{14}$. Then, with $R_i = R(q_i)$, we have*

$$\Gamma_{\mathsf{bcc}}(R_1) \cap \Gamma_{\mathsf{bcc}}(R_2) \;=\; \Gamma_{\mathsf{bcc}}(R_3) \cap \Gamma_{\mathsf{bcc}}(R_4)$$

if and only if $\alpha_1 = \alpha_3$, $\alpha_2 - \alpha_{12} = \alpha_4 - \alpha_{34}$, $\alpha_1 - \alpha_{13} \leqslant \min(\alpha_4 - \alpha_{34}, \alpha_{34})$ and $\alpha_4 - \alpha_{24} \leqslant \min(\alpha_4 - \alpha_{34}, \alpha_{34})$ are satisfied. □

Note that the ordering conditions on the α coefficients do not put any restrictions on the applicability of the theorem, since we can always interchange the role of the q_i such that these conditions are met.

Remark 3.12.5. The two conditions $\alpha_1 = \alpha_3$ and $\alpha_2 - \alpha_{12} = \alpha_4 - \alpha_{34}$ correspond to the two conditions in Lemma 3.12.2. The first one means that the least common multiples of the denominators must be the same, and the second follows from the equality of the indices, which gives $\alpha_1 + \alpha_2 - \alpha_{12} = \alpha_3 + \alpha_4 - \alpha_{34}$. Furthermore, the condition $\alpha_1 - \alpha_{13} \leqslant \alpha_4 - \alpha_{34}$ can easily be understood by considering

$$\begin{aligned} \Gamma_{\mathsf{bcc}}(R_1) \cap \Gamma(R_3) \;&\supseteq\; \Gamma_{\mathsf{bcc}}(R_1) \cap \Gamma_{\mathsf{bcc}}(R_2) \cap \Gamma_{\mathsf{bcc}}(R_3) \cap \Gamma_{\mathsf{bcc}}(R_4) \\ &=\; \Gamma_{\mathsf{bcc}}(R_3) \cap \Gamma_{\mathsf{bcc}}(R_4). \end{aligned}$$ ◊

Theorem 3.12.4 is not very intuitive, but we can understand it better by comparing the quaternions involved. It basically tells us how different the quaternions q_1, q_3 and q_2, q_4 may be; see [97] for details. This allows us to calculate the counting function for MCSLs that are the intersection of at most two ordinary CSLs.

Theorem 3.12.6 ([97, Thm. 6.2.4])**.** *Let p be an odd prime number. Then, the number $c^{(2)}_{\mathsf{bcc}}(p^r)$ of distinct MCSLs of Γ_{bcc} of index p^r that are an intersection of at most two ordinary CSLs is given by*

$$\begin{aligned} c^{(2)}_{\mathsf{bcc}}(p^r) \;=\; &\frac{r+1}{2}\,(p+1)\,p^{r-1} + \left(\frac{r}{2} - 1\right) p^{r-2} - \left(\frac{r}{2} - \left[\frac{r}{2}\right]\right) p^{r-4} \\ &+ \frac{p^{r-1} - p^{r-2[r/3]-1}}{p^2-1} + \frac{p^{4[r/3]-r+2} - p^{4[r/2]-r-2}}{2(p^2-1)}, \end{aligned}$$

where $[x]$ denotes the Gauß bracket. □

As $c^{(2)}_{\mathsf{bcc}}(n)$ is a multiplicative function, we can find an explicit expression for its Dirichlet series generating function as usual.

Theorem 3.12.7. *Let $c^{(2)}_{\mathsf{bcc}}(m)$ be the number of distinct MCSLs of index m that are an intersection of at most two ordinary CSLs. Then, $c^{(2)}_{\mathsf{bcc}}(\Sigma)$ is a multiplicative arithmetic function whose Dirichlet series is given by*

$$\begin{aligned}
\Psi^{(2)}_{\mathsf{bcc}}(s) \;&:=\; \sum_{n=1}^{\infty} \frac{c^{(2)}_{\mathsf{bcc}}(n)}{n^s} \;=\; \prod_{p\in\mathbb{P}\setminus\{2\}} \psi_2(p,s) \\
&=\; \frac{1-2^{1-3s}}{1+2^{-3s}}\,\frac{\zeta(3s-1)\zeta(3s)}{\zeta(6s)}\,\varphi^{(2)}_{\mathsf{bcc}}(s)\,\Psi_{\mathsf{bcc}}(s) \\
&=\; \frac{(1-2^{1-s})(1-2^{1-3s})}{(1+2^{-s})(1+2^{-3s})}\,\frac{\zeta(s-1)\zeta(s)\zeta(3s-1)\zeta(3s)}{\zeta(2s)\zeta(6s)}\,\varphi^{(2)}_{\mathsf{bcc}}(s) \\
&=\; 1+\tfrac{4}{3^s}+\tfrac{6}{5^s}+\tfrac{8}{7^s}+\tfrac{18}{9^s}+\tfrac{12}{11^s}+\tfrac{14}{13^s}+\tfrac{24}{15^s}+\tfrac{18}{17^s}+\tfrac{20}{19^s}+\tfrac{32}{21^s} \\
&\qquad +\tfrac{24}{23^s}+\tfrac{45}{25^s}+\tfrac{76}{27^s}+\tfrac{30}{29^s}+\tfrac{32}{31^s}+\tfrac{48}{33^s}+\tfrac{48}{35^s}+\tfrac{38}{37^s}+\tfrac{56}{39^s}+\cdots,
\end{aligned}$$

where $\psi_2(p,s)$ is the Euler factor corresponding to $c^{(2)}_{\mathsf{bcc}}(p)$, which is given by

$$\psi_2(p,s) \;:=\; \sum_{r=1}^{\infty} \frac{c^{(2)}(p^r)}{p^{rs}} \;=\; \frac{(1+p^{-s})(1+p^{-3s})}{(1-p^{1-s})(1-p^{1-3s})} \times C(p,s)$$

with

$$C(p,s) \;=\; \left(1+\frac{p^{-2s}(p^2+p)}{2(1+p^{-s})(1-p^{1-s})}-\frac{p^{-4s}(p+1)}{(1+p^{-s})(1-p^{1-s})(1+p^{-3s})}\right),$$

while $\varphi^{(2)}_{\mathsf{bcc}}(s)$ is then given by

$$\varphi^{(2)}_{\mathsf{bcc}}(s) \;=\; \prod_{p\in\mathbb{P}\setminus\{2\}} C(p,s),$$

where the product runs over all odd rational primes. □

The explicit knowledge of $\Psi^{(2)}_{\mathsf{bcc}}(s)$ allows us to find its analytic properties. We know from Section 3.9 that $\Psi_{\mathsf{bcc}}(s)$ is meromorphic function of s, whose rightmost pole is located at $s=2$. Furthermore, $\varphi^{(2)}_{\mathsf{bcc}}(s)$ converges absolutely in the half-plane $\left\{\mathrm{Re}(s)>\frac{3}{2}\right\}$, which guarantees its analyticity there. Thus, we get the following asymptotic behaviour.

Corollary 3.12.8 ([97, Cor. 6.2.6])**.** *The asymptotic behaviour of the summatory function of $c^{(2)}_{\mathsf{bcc}}(m)$ is given by*

$$\sum_{m\leqslant x} c^{(2)}_{\mathsf{bcc}}(m) \;\sim\; \frac{\rho^{(2)}_{\mathsf{bcc}}}{2}x^2 \;\approx\; 0.356491\,x^2,$$

as $x \to \infty$, *with*

$$\rho^{(2)}_{\mathsf{bcc}} := \operatorname{res}_{s=2}\bigl(\Psi^{(2)}_{\mathsf{bcc}}(s)\bigr) = \frac{124}{325}\,\frac{\zeta(2)\zeta(6)\zeta(5)}{\zeta(4)\zeta(12)}\,\varphi^{(2)}_{\mathsf{bcc}}(2)$$
$$= \frac{3866940}{691\pi^8}\,\zeta(5)\,\varphi^{(2)}_{\mathsf{bcc}}(2) \approx 0.712983. \qquad \square$$

If we compare the asymptotic growth rates for ordinary CSLs and MCSLs, we see that the latter is not much bigger than the former. This shows that most MCSLs are ordinary CSLs. This behaviour is not surprising, since $c^{(2)}_{\mathsf{bcc}}(m) = c_{\mathsf{bcc}}(m)$ for square-free indices m. Thus, all terms n^{-s} with n square-free are missing in the expansion of $\Psi^{(2)}_{\mathsf{bcc}}(s) - \Psi_{\mathsf{bcc}}(s)$, whose first terms are given by

$$\Psi^{(2)}_{\mathsf{bcc}}(s) - \Psi_{\mathsf{bcc}}(s) = \tfrac{6}{9^s} + \tfrac{15}{25^s} + \tfrac{40}{27^s} + \tfrac{36}{45^s} + \tfrac{28}{49^s} + \tfrac{48}{63^s} + \tfrac{60}{75^s} + \tfrac{174}{81^s} + \tfrac{72}{99^s} + \tfrac{84}{117^s} + \tfrac{66}{121^s} + \tfrac{156}{125^s} + \tfrac{240}{135^s} + \tfrac{112}{147^s} + \tfrac{108}{153^s} + \cdots$$

For the determination of the counting function, it was sufficient to have an explicit expression for $\mathit{\Gamma}_{\mathsf{bcc}}(R_1, R_2)$ for prime power indices. Nevertheless, we can give an explicit expression for MCSLs with general index as well, which generalises Lemma 3.12.3.

Theorem 3.12.9 ([97, Thm. 6.2.7])**.** *Let* q_1 *and* q_2 *be primitive odd quaternions and let* q *be their least common right multiple. Then, one has the relation* $\mathit{\Gamma}_{\mathsf{bcc}}\bigl(R(q_1), R(q_2)\bigr) = \operatorname{Im}(q\mathbb{J} + q_1\mathbb{J}\bar{q}_2) = \operatorname{Im}(q\mathbb{J} + q_2\mathbb{J}\bar{q}_1)$. $\square$

3.12.2. Intersections of three or more CSLs

We can go one step further and analyse MCSLs which are the intersection of at most three ordinary CSLs. Again, it is sufficient to consider only MCSLs of prime power index. Also in this case, we get an explicit expression for the MCSLs as follows.

Theorem 3.12.10 ([97, Thm. 6.3.7])**.** *Let* q_i *with* $i \in \{1, 2, 3\}$ *be odd primitive quaternions with prime power norm* $|q_i|^2 = p^{\alpha_i}$, *such that* $|q_1|^2 \geqslant |q_i|^2$. *Let* $m_{ij} = \operatorname{lcrm}(q_i, q_j)$ *and* $g_{ij} = \operatorname{gcld}(q_i, q_j)$. *Let* $|m_{12}|^2 \geqslant |m_{13}|^2$. *Then,*

$$\mathit{\Gamma}_{\mathsf{bcc}}\bigl(R(q_1), R(q_2), R(q_3)\bigr) = \operatorname{Im}\bigl(m_{12}\mathbb{J} + nq_1\mathbb{J}\bar{q}_2\bigr),$$

where $n = \max\Bigl(1, \frac{|q_3|^2}{|g_{13}|^2|g_{23}|^2}\Bigr)$. $\square$

Note that the expression for the triple CSL in Theorem 3.12.10 is very similar to the expression for the double CSL in Lemma 3.12.3. In fact, the only difference is that an additional factor n occurs. If $n = 1$, the triple CSL is just the intersection of two ordinary CSLs, since one has the relation $\mathit{\Gamma}_{\mathsf{bcc}}(R(q_1), R(q_2), R(q_3)) = \mathit{\Gamma}_{\mathsf{bcc}}(R(q_1), R(q_2)) \subseteq \mathit{\Gamma}_{\mathsf{bcc}}(R(q_1), R(q_3))$ in this case. Let us note in passing that this yields a criterion for the inclusion

$\Gamma\big(R(q_1), R(q_2)\big) \subseteq \Gamma\big(R(q_1), R(q_3)\big)$. In particular, under the assumptions of Theorem 3.12.10, it holds if and only if

$$\frac{|q_3|^2}{|g_{13}|^2\,|g_{23}|^2} \leqslant 1.$$

But even if $n > 1$, the triple CSL is just a multiple of a double CSL, as we have the following result.

Theorem 3.12.11 ([97, Thm. 6.3.8])**.** *Let Γ' be a sublattice of Γ_{bcc} of prime power index p^α. Then, Γ' can be represented as the intersection of three ordinary CSLs,*

$$\Gamma' \,=\, \Gamma_{\mathsf{bcc}}(R_1) \cap \Gamma_{\mathsf{bcc}}(R_2) \cap \Gamma_{\mathsf{bcc}}(R_3),$$

if and only if there exists $\beta \in \mathbb{N}_0$ together with two coincidence rotations R_1' and R_2' such that $\Gamma' = p^\beta(\Gamma_{\mathsf{bcc}}(R_1') \cap \Gamma_{\mathsf{bcc}}(R_2'))$. The integer β is determined uniquely by Γ'. □

Thus, we have established a one-to-one correspondence between intersections of three ordinary CSLs and multiples of intersections of two ordinary CSLs. This allows us to express $c^{(3)}_{\mathsf{bcc}}(p^r)$ in terms of $c^{(2)}_{\mathsf{bcc}}(p^r)$ as follows.

Corollary 3.12.12 ([97, Cor. 6.3.9])**.** *Let p be an odd prime number. Then,*

$$c^{(3)}_{\mathsf{bcc}}(p^r) \,=\, \sum_{0 \leqslant n \leqslant r/3} c^{(2)}_{\mathsf{bcc}}(p^{r-3n}),$$

where $c^{(3)}_{\mathsf{bcc}}(m)$ and $c^{(2)}_{\mathsf{bcc}}(m)$ denote the number of MCSLs of index m that can be written as an intersection of (up to) three and two ordinary CSLs, respectively. □

As $c^{(3)}_{\mathsf{bcc}}$ is once again multiplicative, we can easily infer its generating function as follows.

Theorem 3.12.13 ([97, Thm. 6.3.10])**.** *Let $c^{(3)}_{\mathsf{bcc}}(m)$ be the number of distinct MCSLs of index m that are an intersection of at most three ordinary CSLs. Then, $c^{(3)}_{\mathsf{bcc}}(m)$ is a multiplicative arithmetic function whose Dirichlet series is given by*

$$\Psi^{(3)}_{\mathsf{bcc}}(s) \,:=\, \sum_{n=1}^{\infty} \frac{c^{(3)}_{\mathsf{bcc}}(n)}{n^s} \,=\, (1 - 2^{-3s})\,\zeta(3s)\,\Psi^{(2)}_{\mathsf{bcc}}(s)$$

where $\Psi^{(2)}_{\mathsf{bcc}}(s)$ is given by Theorem 3.12.7*. One finds*

$$\begin{aligned}\Psi^{(3)}_{\mathsf{bcc}}(s) \,=\, 1 &+ \tfrac{4}{3^s} + \tfrac{6}{5^s} + \tfrac{8}{7^s} + \tfrac{18}{9^s} + \tfrac{12}{11^s} + \tfrac{14}{13^s} + \tfrac{24}{15^s} + \tfrac{18}{17^s} + \tfrac{20}{19^s} + \tfrac{32}{21^s} \\ &+ \tfrac{24}{23^s} + \tfrac{45}{25^s} + \tfrac{77}{27^s} + \tfrac{30}{29^s} + \tfrac{32}{31^s} + \tfrac{48}{33^s} + \tfrac{48}{35^s} + \tfrac{38}{37^s} + \tfrac{56}{39^s} + \cdots\end{aligned}$$

for the leading terms. □

Familiar arguments involving Theorem 3.4.1 yield the following asymptotic behaviour.

Corollary 3.12.14 ([97, Cor. 6.3.11]). *The asymptotic behaviour of the summatory function of $c^{(3)}_{\mathsf{bcc}}(m)$, as $x \to \infty$, is given by*

$$\sum_{m \leqslant x} c^{(3)}_{\mathsf{bcc}}(m) \;=\; \frac{\rho^{(3)}_{\mathsf{bcc}}}{2}\, x^2 \;\approx\; 0.357007\, x^2,$$

where

$$\begin{aligned}\rho^{(3)}_{\mathsf{bcc}} \,:= \operatorname{res}_{s=2}\bigl(\Psi^{(3)}_{\mathsf{bcc}}(s)\bigr) \;&=\; \frac{63}{64}\,\zeta(6)\,\rho^{(2)}_{\mathsf{bcc}} \;=\; \frac{1953}{5200}\,\frac{\zeta(2)\zeta(6)^2\zeta(5)}{\zeta(4)\zeta(12)}\,\varphi^{(2)}_{\mathsf{bcc}}(2) \\ &=\; \frac{64449}{11056\pi^2}\,\zeta(5)\,\varphi^{(2)}_{\mathsf{bcc}}(2) \;\approx\; 0.714014. \qquad \square\end{aligned}$$

Comparing these results with Corollary 3.12.8, we see that the difference in the growth rate is significantly below 1%. This small difference is not surprising as genuinely triple CSLs can only occur for indices that are divisible by p^3 for some odd p. In particular, the first such lattice occurs for the index $\Sigma = 27$. The fact that new MCSLs are rather rare is also illustrated by the first terms of the expansion

$$\begin{aligned}\Psi^{(3)}_{\mathsf{bcc}}(s) - \Psi^{(2)}_{\mathsf{bcc}}(s) \;&=\; \Psi^{(2)}_{\mathsf{bcc}}(s)\,\bigl((1-2^{-3s})\zeta(3s)-1\bigr) \\ &=\; \tfrac{1}{27^s} + \tfrac{4}{81^s} + \tfrac{1}{125^s} + \tfrac{6}{135^s} + \tfrac{8}{189^s} + \tfrac{18}{243^s} + \tfrac{12}{297^s} + \tfrac{1}{343^s} + \tfrac{14}{351^s} + \cdots\end{aligned}$$

Here, all terms n^{-s} with n cube-free are missing, which is just a reformulation of the fact that $c^{(3)}_{\mathsf{bcc}}(n) = c^{(2)}_{\mathsf{bcc}}(n)$ for these n.

Finally, let us mention that any triple CSL is just a multiple of a double CSL for general index m, as we have the following generalisation of Theorem 3.12.11.

Theorem 3.12.15 ([97, Thm. 6.3.12]). *Let R_i with $i \in \{1,2,3\}$ be coincidence rotations of $\varGamma_{\mathsf{bcc}}$. Then, there exist rotations R'_1 and R'_2 together with an integer $n \in \mathbb{N}$ such that $\varGamma_{\mathsf{bcc}}(R_1,R_2,R_3) = n\varGamma_{\mathsf{bcc}}(R'_1,R'_2)$. Conversely, for any sublattice of the form $n\varGamma_{\mathsf{bcc}}(R'_1,R'_2)$, there exist coincidence rotations R_i with $i \in \{1,2,3\}$ such that $\varGamma_{\mathsf{bcc}}(R_1,R_2,R_3) = n\varGamma_{\mathsf{bcc}}(R'_1,R'_2)$.* $\square$

In fact, this yields all MCSLs, as any MCSL of $\varGamma_{\mathsf{bcc}}$ can be written as the intersection of three ordinary CSLs.

Theorem 3.12.16 ([97, Thm. 6.4.3]). *Let $R_1,\ldots,R_n$ be a finite number of coincidence rotations of $\varGamma_{\mathsf{bcc}}$. Then, there exist coincidence rotations R'_1, R'_2 and R'_3 such that $\varGamma_{\mathsf{bcc}}(R_1,\ldots,R_n) = \varGamma_{\mathsf{bcc}}(R'_1,R'_2,R'_3)$.* $\square$

Consequently, no new MCSLs emerge if we consider intersections of more than three ordinary CSLs. Hence, the total number of MCSLs of given index

m is already given by $c^{(3)}_{\mathsf{bcc}}(m)$, which means that, for all $n \geqslant 3$, we have

$$c^{(\infty)}_{\mathsf{bcc}}(m) \,=\, c^{(n)}_{\mathsf{bcc}}(m) \,=\, c^{(3)}_{\mathsf{bcc}}(m).$$

A similar phenomenon has been observed in two dimensions, where the set of MCSLs stabilises already for $n = 2$; compare Section 3.8 and [8].

So far, we have only discussed the body-centred cubic lattice. However, we know from the ordinary CSLs that all three types of cubic lattices have the same group of coincidence rotations, the same spectrum of indices and the same multiplicity function. In fact, this remains true in the case of MCSLs, too; compare [97, Thms. 6.5.2, 6.5.4 and 6.5.5].

Theorem 3.12.17. *Let $R_1, \ldots, R_n$ be coincidence rotations for the cubic lattices in the setting of Eq.* (3.9.1)*. Then,*

$$\Sigma_{\mathsf{pc}}(R_1, \ldots, R_n) \,=\, \Sigma_{\mathsf{bcc}}(R_1, \ldots, R_n) \,=\, \Sigma_{\mathsf{fcc}}(R_1, \ldots, R_n).$$

Moreover,

$$\varGamma_{\mathsf{pc}}(R_1, \ldots, R_n) \,=\, \varGamma_{\mathsf{bcc}}(R_1, \ldots, R_n) \cap \varGamma_{\mathsf{pc}} \quad \text{and}$$

$$\varGamma_{\mathsf{fcc}}(R_1, \ldots, R_n) \,=\, \varGamma_{\mathsf{bcc}}(R_1, \ldots, R_n) \cap \varGamma_{\mathsf{fcc}}$$

relate the CSLs of the different cubic lattices. □

This result implies that the counting functions are equal for all three cubic lattices, too. In particular, we have

$$c^{(n)}_{\mathsf{pc}}(m) \,=\, c^{(n)}_{\mathsf{fcc}}(m) \,=\, c^{(n)}_{\mathsf{bcc}}(m) \tag{3.12.2}$$

for any $n \in \mathbb{N} \cup \{\infty\}$, and the corresponding generating functions are equal as well.

Finally, let us mention an application to crystallography. One object of interest to crystallographers are so-called triple junctions [40, 39, 41]. Roughly speaking, *triple junctions* are three crystal grains meeting in a straight line. This means that there are three pairs of grains sharing a common plane (grain boundary). They give rise to three simple CSLs and to a double CSL, which is the intersection of the former. In our terms, the latter is an MCSL $\varGamma \cap R_1\varGamma \cap R_2\varGamma$, whereas the former are the simple CSLs $\varGamma \cap R_1\varGamma$, $\varGamma \cap R_2\varGamma$ and $R_1\varGamma \cap R_2\varGamma$, respectively. An important question is the relation of the indices of these lattices.

Let us denote the indices of the simple CSLs by $\Sigma_i := \Sigma(R_i)$, where $R_3 := R_1^{-1}R_2$. Let q_1 and q_2 be the quaternions that parametrise R_1 and R_2, respectively. Then, R_3 is generated by $\bar{q}_1 q_2$, which is not a primitive quaternion in general. The corresponding primitive quaternion is given by $q_3 := \frac{\bar{q}_1 q_2}{|q_{12}|^2}$, where $q_{12} = \mathrm{gcld}(q_1, q_2)$. Hence, we can immediately reproduce Gertsman's result [39] for the index $\Sigma_3 = \frac{\Sigma_1 \Sigma_2}{\Sigma_{12}^2}$, where $\Sigma_{12} := \Sigma(R(q_{12}))$ is

the index that corresponds to the rotation $R(q_{12})$. On the other hand, we know from Lemma 3.7.14 and Eq. (3.12.1) that

$$\Sigma(R_1, R_2) \;=\; \frac{\Sigma_1\Sigma_2}{\Sigma_{12}} \;=\; \Sigma_{12}\,\Sigma_3.$$

Now, we define $q_1' := q_{12}^{-1}q_1$ and $q_2' := q_{12}^{-1}q_2$. Then, we may write

$$q_1 \;=\; q_{12}q_1', \quad q_2 \;=\; q_{12}q_2', \quad q_3 \;=\; \bar{q}_1'q_2' \tag{3.12.3}$$

and, correspondingly, we may decompose the rotations R_i into the 'basic' constituents $R_{12} := R(q_{12})$, $R_1' := R(q_1')$ and $R_2' := R(q_2')$. We note that the corresponding indices are multiplicative,

$$\Sigma(R_1) \;=\; \Sigma(R_{12})\Sigma(R_1'),\; \Sigma(R_2) \;=\; \Sigma(R_{12})\Sigma(R_2'),\; \Sigma(R_3) \;=\; \Sigma(R_1')\Sigma(R_2').$$

Furthermore, we see $\bar{q}_1' \;=\; \gcld(\bar{q}_1, q_3) =: q_{13}$ and $\bar{q}_2' \;=\; \gcld(\bar{q}_2, \bar{q}_3) =: q_{23}$, whence Eq. (3.12.3) may be written in a more symmetric way as

$$q_1 \;=\; q_{12}\bar{q}_{13} \;=\; \frac{q_2\bar{q}_3}{|q_{23}|^2}, \quad q_2 \;=\; q_{12}\bar{q}_{23} \;=\; \frac{q_1q_3}{|q_{13}|^2}, \quad q_3 \;=\; \bar{q}_{13}\bar{q}_{23} \;=\; \frac{\bar{q}_1q_2}{|q_{12}|^2}.$$

If we define the corresponding indices in the obvious way, we see that the index $\Sigma(R_1, R_2)$ can be written as

$$\begin{aligned}\Sigma(R_1, R_2) \;&=\; \frac{\Sigma_1\Sigma_2}{\Sigma_{12}} \;=\; \frac{\Sigma_1\Sigma_3}{\Sigma_{13}} \;=\; \frac{\Sigma_2\Sigma_3}{\Sigma_{23}} \;=\; \Sigma_{12}\Sigma_3 = \Sigma_{13}\Sigma_2 = \Sigma_{23}\Sigma_1 \\ &=\; \Sigma_{12}\Sigma_{13}\Sigma_{23} \;=\; \Sigma_{12}\Sigma_1'\Sigma_2' \;=\; \bigl(\Sigma_1\Sigma_2\Sigma_3\bigr)^{\frac{1}{2}}.\end{aligned}$$

The last expression was proved by different methods in [39]. Note that we can express $\Sigma(R_1, R_2)$ either in terms of the simple indices $\Sigma_1, \Sigma_2, \Sigma_3$ or in terms of the 'reduced' indices $\Sigma_{12}, \Sigma_{13}, \Sigma_{23}$, which somehow describe the 'common' part of R_1, R_2 and R_3. Note that R_{12}, R_{13} and R_{23} contain the complete information about the triple junction. In particular, we can write $\Gamma(R_1, R_2)$ as $\Gamma(R_1, R_2) = R_{12}(R_{12}^{-1}\Gamma \cap R_{13}^{-1}\Gamma \cap R_{23}^{-1}\Gamma)$.

As we have now solved the problem of MCSLs of the cubic lattices, it is natural to ask whether these results can be generalised. Unfortunately, not much is known about MCSLs in dimensions $d > 3$, not even for the A_4-lattice or the hypercubic lattices. This is not too surprising in view of the fact that the computation of MCSLs is substantially more difficult than the determination of ordinary CSLs. Indeed, even for the 4-dimensional root lattices, no explicit expression for the MCSLs is known, which makes the corresponding enumeration problem intractable along the explicit route we have taken above.

Still, there are several interesting questions to address. A striking feature of our examples is the stabilisation property of the coincidence spectra and of the MCSLs themselves. For the planar lattices and modules of Section 3.8,

any MCSM can be represented as the intersection of at most two ordinary CSMs, whereas for the cubic lattices up to three ordinary CSLs are needed. One might suspect that, in dimension d, any MCSL can be written as the intersection of at most d ordinary CSLs, but this seems too difficult to decide at the moment.

A somewhat easier problem is the stabilisation phenomenon of the coincidence spectra. For the cubic lattices as well as for the planar lattices and modules of Section 3.8, we have $\sigma_\infty(\varGamma) = \sigma(\varGamma)$; compare Proposition 3.12.1 and Eq. (3.8.8). Similarly, we have $\sigma_\infty(\varGamma) = \sigma(\varGamma)$ for the lattices A_4, D_4^* and $\mathbb{Z}^4$. For A_4 and D_4^*, this follows immediately from $\sigma(\varGamma) = \widehat{\sigma}(\varGamma)$ and Eq. (3.7.3). For $\mathbb{Z}^4$, one has to argue differently, as $\sigma(\varGamma) \neq \widehat{\sigma}(\varGamma)$. Here, index considerations similar to those in Eq. (3.10.12) do the job.

There are two further (somewhat extremal) situations where we can prove stabilisation. If the simple spectrum is a finite set, which is equivalent to the finiteness of the set of CSLs, the coincidence spectra must stabilise after a finite number of steps, as the set of all MCSLs is finite as well. This happens for the rather large class of planar lattices that have exactly two coincidence reflections; compare [18]. The second situation is the case $\sigma(\varGamma) = \mathbb{N}$, where we obviously have $\sigma_\infty(\varGamma) = \sigma(\varGamma)$. This happens for $\varGamma = \mathbb{Z}^d$ for $d \geqslant 5$, as we shall see below.

3.13. Results in higher dimensions

For dimensions $d \geqslant 4$, not much is known about CSLs in general, let alone CSMs. However, if $\varGamma$ is *rational*, we have some results on the possible indices. In this case, the group $\mathrm{OC}(\varGamma)$ is generated by coincidence reflections. To be more concrete, let $R_v \colon \mathbb{R}^d \longrightarrow \mathbb{R}^d$, $x \mapsto x - 2\frac{\langle v|x\rangle}{\langle v|v\rangle}v$ denote the reflection in the plane perpendicular to $v \in \mathbb{R}^d$. As a first result, we mention the following characterisation of rational lattices.

Theorem 3.13.1 ([98, Thm. 3.2 and Cor. 3.3])**.** *A lattice $\varGamma \subset \mathbb{R}^d$ is rational*[11] *if and only if any reflection R_v with $v \in \varGamma \setminus \{0\}$ is a coincidence reflection.* □

As we have plenty of coincidence reflections for rational lattices, it is not a surprise that they generate the group $\mathrm{OC}(\varGamma)$. In particular, we have the following analogue of the classic Cartan–Dieudonné theorem (see [22, 38]) for coincidence isometries.

Theorem 3.13.2 ([98, Thm. 3.1 and Thm. 3.5])**.** *Let $\varGamma \subset \mathbb{R}^d$ be a rational lattice (in the wider sense). Then, any coincidence isometry of $\varGamma$ is a product of at most d coincidence reflections generated by lattice vectors of $\varGamma$.* □

[11] meaning rational in the wider sense; compare Footnote 4 on page 98.

Theorem 3.13.2 allows us to determine the coincidence spectrum for some rational lattices. As an example, we consider $\Gamma = \mathbb{Z}^d$. In this case, $\mathrm{OC}(\mathbb{Z}^d)$ is generated by the reflections R_v, where v runs through all non-zero primitive lattice vectors. The coincidence index $\Sigma(R_v)$ can be calculated explicitly and, for primitive v, is given by [99, Thm. 3.2] as

$$\Sigma(R_v) = \begin{cases} \langle v|v\rangle, & \text{if } \langle v|v\rangle \text{ is odd,} \\ \frac{1}{2}\langle v|v\rangle, & \text{if } \langle v|v\rangle \text{ is even.} \end{cases} \tag{3.13.1}$$

As any positive integer n can be written as the sum of four squares, there exists a primitive vector $v \in \mathbb{Z}^d$ with $\langle v|v\rangle = 2n$ for $d \geqslant 5$ (choose one of the components to be 1, which guarantees the primitivity, and adjust the other components to get length $\langle v|v\rangle = 2n$). Hence, in $\mathbb{Z}^d$ with $d \geqslant 5$, all positive integers occur as a coincidence index of some reflection, which gives us the coincidence spectrum; compare [99].

Fact 3.13.3. *The coincidence spectrum of $\mathbb{Z}^d$ for $d \geqslant 5$ is $\mathbb{N}$.* □

Remark 3.13.4. Previously, we have seen that the coincidence spectrum of $\mathbb{Z}^d$ is a proper subset of $\mathbb{N}$ for $2 \leqslant d \leqslant 4$; compare Example 3.8.5 and Remarks 3.9.6 and 3.10.12. Although Theorem 3.13.2 guarantees that the coincidence reflections generate $\mathrm{OC}(\mathbb{Z}^d)$, it is not evident whether they yield the whole coincidence spectrum. But, in fact, this is indeed the case. Moreover, for $2 \leqslant d \leqslant 4$, it follows that n is the index of a coincidence reflection if and only if n is the index of a coincidence rotation.

This is obvious for $d = 2$, as there is an index-preserving bijection between coincidence reflections and coincidence rotations (observe that any reflection is the product of complex conjugation with a rotation).

For $d = 3$ or $d = 4$, there is no such bijection. Nevertheless, we get the possible indices for coincidence reflections by evaluating Eq. (3.13.1). This is straightforward for $d = 4$, where we conclude that exactly all odd positive integers and all positive integers of the form $4n + 2$ occur as coincidence indices for some coincidence reflection. These are the same indices we found for the coincidence rotations of $\mathbb{Z}^4$ in Section 3.10; compare Remark 3.10.12.

For $d = 3$, evaluating Eq. (3.13.1) is more difficult. Recall that any integer that is not of the form $4^k m$ with $m \equiv 7 \bmod 8$ can be written as the sum of three squares. Hence, for any odd n, there exists a vector $v \in \mathbb{Z}^3$ such that $\langle v|v\rangle = 2n$. In fact, there even exists a primitive v, since a positive integer $m \not\equiv 0 \bmod 4$ can be represented as a sum of three integers if and only if it has a primitive representation; see [28] for an explicit formula for the number of primitive representations. Thus, there is a coincidence reflection of index n for any positive odd n. Recall from Section 3.9 that there are coincidence rotations of index n for all positive odd n as well. ◊

Theorem 3.13.1 can be generalised to $\mathcal{S}$-lattices, as its proof is algebraic in nature. The analogue of a rational lattice can be characterised as follows.

Theorem 3.13.5 ([56, Thm. 3.2]). *Let $M \subseteq \mathbb{R}^d$ be an $\mathcal{S}$-lattice, and let K be the field of fractions of $\mathcal{S}$. Then, the following properties are equivalent.*

(1) *For all $u, v \in M$ and $w \in M \setminus \{0\}$, we have $\frac{\langle u \,|\, v\rangle}{\langle w \,|\, w\rangle} \in K$;*
(2) *R_v is a coincidence reflection for any $v \in M \setminus \{0\}$.* □

For any $\mathcal{S}$-lattice that satisfies the properties of Theorem 3.13.5, we have the following generalisation of Theorem 3.13.2, which again is an analogue of the Cartan–Dieudonné theorem.

Theorem 3.13.6 ([56, Thm. 3.1]). *Let $M \subseteq \mathbb{R}^d$ be an $\mathcal{S}$-lattice, and let K be the field of fractions of $\mathcal{S}$. Let M satisfy the conditions of Theorem* 3.13.5. *Then, any coincidence isometry of M can be written as the product of at most d coincidence reflections generated by non-zero vectors of M.* □

To get more concrete results in dimensions $d \geqslant 5$, it would be nice to have an explicit parametrisation for the coincidence isometries. For dimensions $d = 3$ and $d = 4$, we profitted from the parametrisation of rotation by quaternions. An obvious candidate for higher dimensions is Cayley's parametrisation of rotations in terms of Clifford algebras. At present, however, we are not aware of any concrete results in this direction for $d \geqslant 5$.

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CHAPTER 4

Almost Periodic Measures and their Fourier Transforms

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The theory of almost periodic measures and their Fourier transforms underlies the mathematics of diffraction, particularly as it applies to the study of long-range non-periodic and aperiodic order. This chapter presents a streamlined development of the theory, tailored to this purpose. Our exposition expands on Chapters 8 and 9 of [AO1]. To keep the presentation self-contained, all important terms and concepts are explicitly introduced and defined.

4.1. Introduction

Long-range non-periodic order is not a particularly well-defined notion, but broadly it refers to structures, mathematical and physical, that are not fully periodic (or crystallographic) but still have the property that local environments, even when widely separated, are correlated with one another.

An important indicator of long-range order is *diffraction*, because diffraction is a physically accessible attribute of materials that depends on the global structure, and it is also good at indicating repetitions of local motives. Regular translational repetition of structural elements appears in diffraction as *Bragg peaks* (atomic or pure point parts of the measure). A common situation in crystallography, and in the study of quasicrystals and other related aperiodic crystal-like structures, is the appearance of a relatively dense set of Bragg peaks, including the situation in which the diffraction consists entirely of Bragg peaks (pure point diffraction). For a thorough introduction to aperiodic order and to diffraction from aperiodic structures, we refer the reader to the flagship volume of this series, [AO1].

From a mathematical point of view, the diffraction of a structure in $\mathbb{R}^d$ is a measure on the Fourier dual space (which is another copy of $\mathbb{R}^d$) that is positive (and often positive definite, too). It is obtained as the Fourier transform of another measure, which is positive definite (and often positive, too), called the *autocorrelation* or 2-point correlation measure of the structure. In

the case of crystals, many of the underlying subtleties of the mathematics of diffraction are ameliorated, because the Bragg peaks are nicely spaced on a lattice and because the group of translational symmetries of the crystal allows the *Poisson summation formula* (PSF) to be used to determine the Fourier transformation. In the aperiodic case, things are not as simple (though the PSF is vital in this context, too [39]). Bragg peaks can be dense in Fourier space, and convergence issues become important. Thus, unfortunately, at the very start of the subject of long-range aperiodic order, one is faced with issues that are subtle and prone to many confusions and even downright errors. To get this all straight, one requires a deeper understanding of the mathematics of unbounded measures and their Fourier transforms.

Ultimately, we shall see that long-range order, as seen from the perspective of diffraction, is Fourier-dual to a suitable concept of *almost periodicity* within the structure itself. So, the real work becomes that of understanding almost periodic functions and almost periodic measures, along with their Fourier transforms. The principal setting is that of weakly almost periodic functions. The key results are of the form that characterise pure point diffraction (respectively continuous diffraction) with strong (respectively null weak) almost periodicity of the Fourier transform. Specifically,

- measures on $\mathbb{R}^d$ that are both positive and positive definite are Fourier transformable and weakly almost periodic; their Fourier transforms are also positive and positive definite;
- every Fourier transformable measure is a weakly almost periodic measure, and is uniquely decomposable as the sum of a strongly almost periodic measure and a null weakly almost periodic measure;
- a Fourier transformable measure is strongly almost periodic (respectively null weakly almost periodic) if and only if its Fourier transform is a pure point (respectively continuous) measure.

These results are the content of Theorems 4.10.4, 4.10.10, 4.10.12 and 4.11.7, and of Corollary 4.11.6.

The principal reference for this work is the exposition by Gil de Lamadrid and Argabright [19], which, one may say, is devoted essentially to deriving the results that we have just stated. There, the results are set in a more general context than we need and the reader is supposed to have a good background in the theory of almost periodic functions. Our objective here is clear: To offer a straightforward and fairly self-contained development of the theory of almost periodic functions and measures which will be adequate for the theory of diffraction in the study of long-range order.

Although the main applications are to structures in real spaces, it is well known that in the cut and project formalism, so prevalent in the theory of

quasicrystals, more general types of *locally compact Abelian groups* (LCAGs) appear rather naturally. Working over these more general groups rather than real spaces does not increase the level of difficulty or abstraction required for the theory, and in one way or another will most likely be required in the subject anyway. For this reason, the setting of this chapter is locally compact Abelian groups.

We would be remiss if we did not mention at this point that the whole notion of what it means to be almost periodic depends on what topology one wishes to use to define it. We study here the definition that has been found to be appropriate for diffraction, and this relates to almost periodicity of the autocorrelation. But, within the field of aperiodic order, there are significant uses of almost periodic measures that are applied in other ways to the physical or mathematical distributions of the structure of interest; see for example [20, 27, 18, 30, 33], and Chapter 5 in this volume [46].

This chapter is organised as follows. In Section 4.2, we start by reviewing Pontryagin duality and Bohr compactification for LCAGs. Then, in Sections 4.3–4.6, we review the theory of almost periodic functions, amenability, Eberlein's ergodic theorem and Eberlein convolution. Our exposition in these sections follows closely that given in [15]. We continue by reviewing the decomposition of weakly almost periodic functions into strong and null weakly almost periodic parts, as introduced in [17].

In Section 4.8, we summarise the theory of Fourier transforms of finite measures, and the connection between the Fourier transforms of finite measures and almost periodicity given in [16]. Next, in Section 4.9, we review the theory of Fourier transformable measures. Here, our approach closely follows the exposition in [1].

In Section 4.10, we review the theory of almost periodic measures. Our approach is simpler than the one in [19], as we do not need the entire generality of their results. We also prove two new results in Theorems 4.10.4 and 4.10.12, which are similar to the corresponding results of [19], but directed in a form more useful for the theory of mathematical diffraction. We complete our survey by reviewing the Fourier transformability of positive definite measures in Section 4.11, where we closely follow [5].

The remainder of this Introduction explains the basic concepts and ideas that form the basis of the theory.

4.1.1. Bohr's theory of almost periodic functions

Harald Bohr's original definition of almost periodic functions on the line is set in the context of the space $C_{\mathsf{u}}(\mathbb{R})$ of all bounded and uniformly continuous $\mathbb{C}$-valued functions on the real line $\mathbb{R}$. This space is equipped with the

topology of the supremum norm (or sup-norm for short); see Section 4.1.2 as well as [AO1, Sec. 8.2].

Definition 4.1.1. Let $f \in C_{\mathsf{u}}(\mathbb{R})$. For $\varepsilon > 0$, $t \in \mathbb{R}$ is an *ε-almost period* of f if, for all $x \in \mathbb{R}$,

$$|f(x+t) - f(x)| < \varepsilon.$$

The function f is *almost periodic* if, for all $\varepsilon > 0$, its set of ε-almost periods is relatively dense[1] in $\mathbb{R}$.

Some of Bohr's main results can be summarised as follows [6].

(i) The space $\mathcal{F}$ of all almost periodic functions in $C_{\mathsf{u}}(\mathbb{R})$ is a closed subspace of $C_{\mathsf{u}}(\mathbb{R})$.

(ii) Every trigonometric polynomial (or sum)

$$a_1 \mathrm{e}^{2\pi \mathrm{i} k_1 x} + \cdots + a_n \mathrm{e}^{2\pi \mathrm{i} k_n x},$$

where $k_1, \ldots, k_n$ are arbitrary (distinct) real numbers and where $a_1, \ldots, a_n \in \mathbb{C}$, is almost periodic as a function of x.

(iii) Every element of $\mathcal{F}$ is the uniform limit of a sequence of trigonometric polynomials as defined in (ii).

(iv) Every element $f \in \mathcal{F}$ has an expansion (its Fourier–Bohr series) in the form

$$f \sim \sum_n a_n \mathrm{e}^{2\pi \mathrm{i} k_n x}.$$

Here, the sum on the right is finite or countably infinite and $\sim$ means that the series convergences to f in the mean (see Definition 4.1.6 and the material around Definition 4.6.5 for details on this).

Intuitively, the connection between almost periodicity of a function and the pure point nature[2] of its Fourier transform is easy to see. If $\widehat{\eta}$ is a pure point measure, one has $\widehat{\eta} = \sum_{j=1}^{\infty} a_j \delta_{k_j}$ and η should thus be $\sum_{j=1}^{\infty} a_j \mathrm{e}^{2\pi \mathrm{i} k_j x}$. The pure point nature of the Fourier transform is then directly related to the approximation of the original measure by trigonometric polynomials. The question is whether or not this kind of formal manipulation makes any mathematical sense.

An important development in the understanding of almost periodic functions was the realisation by S. Bochner of almost periodicity in terms of compactness. If we consider the set $T_{\mathbb{R}} f$ of all translates $T_x f$ of f, with

[1] A subset A of an LCAG G is *relatively dense* if there is a compact set K so that $\bigcup_{a \in A} a + K = G$; compare [AO1, Sec. 2.1]. In $\mathbb{R}$, this means that A is unbounded above and below, and the intervals of $\mathbb{R}$ that are empty of elements of A are bounded in length.

[2] Often, this is called *discreteness* or *atomic nature* in mathematics. Since both words have a different meaning in the context of aperiodic order, we use the term *pure point* instead, as is common in spectral theory.

$x \in \mathbb{R}$ (where $(T_x f)(y) := f(-x+y)$ for all $y \in \mathbb{R}$) then $f \in C_{\mathsf{u}}(\mathbb{R})$ is almost periodic if and only if the closure of $T_{\mathbb{R}} f$ in $C_{\mathsf{u}}(\mathbb{R})$ is compact; see Proposition 4.3.2 below. Bochner's condition is often easier to work with and provides a convenient way to define almost periodicity. This is the approach that we shall use below.

4.1.2. Locally compact Abelian groups and almost periodicity

Our basic objective is to study almost periodic functions and measures in the context of locally compact Abelian groups. The most important examples of such groups are the real spaces $\mathbb{R}^d$, where the group structure is addition. Because of this, we usually find it more convenient to write things in additive notation. However, in the general theory of LCAGs, it is also customary to write the group structure in multiplicative form. Thus, we shall use both forms, but try to avoid any confusion around this.

We shall use the familiar symbols $C(G)$, $C_{\mathsf{c}}(G)$, $C_{\mathsf{u}}(G)$ and $C_0(G)$ for the spaces of continuous, compactly supported continuous, bounded uniformly continuous, and vanishing-at-infinity continuous functions on an LCAG G, respectively. For any function g on G, the functions $\widetilde{g}$ and $g^\dagger$ are defined by

$$\widetilde{g}(x) = \overline{g(-x)} \quad \text{and} \quad g^\dagger(x) = g(-x).$$

For measures μ on G, we define $\widetilde{\mu}$ and $\mu^\dagger$ by

$$\widetilde{\mu}(g) = \overline{\mu(\widetilde{g})} \quad \text{and} \quad \mu^\dagger(g) = \mu(g^\dagger).$$

Here, we use $\mu(g)$ as shorthand for $\int_G g \, \mathrm{d}\mu$.

> **Note.** *Throughout this chapter, G will always denote a locally compact (Hausdorff) Abelian group, or LCAG for short. All measures are assumed to be Radon measures or, equivalently, elements of the dual space of $C_{\mathsf{c}}(G)$; see Definition* 4.9.1 *for more details.*

The group G carries a Haar measure, namely an invariant and positive regular measure, which is unique up to scaling. We choose one such measure $\theta = \theta_G$ once and for all. If G is compact, we shall assume that the Haar measure is chosen to give total measure 1 to G, hence $\theta_G(G) = 1$. In writing integrals, we shall often suppress the explicit symbol of the Haar measure, so one will see

$$\int_G f(t) \, \mathrm{d}t \quad \text{instead of} \quad \int_G f(t) \, \mathrm{d}\theta_G(t).$$

The space $C_{\mathsf{u}}(G)$ of uniformly continuous and bounded $\mathbb{C}$-valued functions on G becomes a Banach space under the sup-norm $\|.\|_\infty$, defined as

$$\|f\|_\infty := \sup\bigl\{|f(x)| : x \in G\bigr\}$$

for $f \in C_{\mathsf{u}}(G)$.

Definition 4.1.2. The *strong topology* on $C_{\mathsf{u}}(G)$ is the topology defined by the sup-norm.

In addition to the strong topology, $C_{\mathsf{u}}(G)$ carries a weak topology. If ϕ is a continuous linear functional on $(C_{\mathsf{u}}(G), \|.\|_\infty)$, we define a semi-norm $\|.\|_\phi$ on $C_{\mathsf{u}}(G)$ by $\|f\|_\phi = |\phi(f)|$.

Definition 4.1.3. The *weak topology* on $C_{\mathsf{u}}(G)$ is the uniform topology defined by the family of semi-norms $\|.\|_\phi$, where ϕ runs through the space $C_{\mathsf{u}}(G)'$ of all continuous (in the strong topology) linear functionals on $C_{\mathsf{u}}(G)$.

This means that the topology is defined from the *uniformity* whose entourages are generated by the sets

$$U[\Phi;\varepsilon] := \big\{(f,g) \in C_{\mathsf{u}}(G)\times C_{\mathsf{u}}(G) : \|f-g\|_\phi < \varepsilon \text{ for all } \phi \in \Phi\big\} \tag{4.1.1}$$

for all $\varepsilon > 0$ and for all *finite* subsets Φ of $C_{\mathsf{u}}(G)'$. We shall use the symbol w-lim to indicate limits taken in the weak topology. Here and below, we employ the language of uniformities; see [8, 23, 49] for background material.

Defining $\|\phi\|_\infty := \sup_{\|f\|_\infty=1} |\phi(f)|$, we obtain the useful facts that, for all $f \in C_{\mathsf{u}}(G)$,

$$\begin{aligned} \|f\|_\phi &\leqslant \|\phi\|_\infty \|f\|_\infty, \quad \text{for all } \phi \in C_{\mathsf{u}}(G)', \\ \|f\|_\infty &= \sup_{\substack{\phi\in C_{\mathsf{u}}(G)' \\ \|\phi\|_\infty=1}} \|f\|_\phi, \end{aligned}$$

and also that the mapping

$$\mathrm{id}\colon C_{\mathsf{u}}(G)_{\mathrm{strong}} \longrightarrow C_{\mathsf{u}}(G)_{\mathrm{weak}} \tag{4.1.2}$$

is continuous.

For each $t \in G$, we define the translation action T_t on G by $T_t(x) = t + x$ for all $x \in G$. This action of G on itself extends in the usual way to an action, also denoted by T, of G on functions on G, namely $f \mapsto T_t f$ with

$$(T_t f)(x) := f(T_t^{-1}x) = f(T_{-t}x) = f(x-t).$$

It is convenient to shorten the notation $T_t f$ to $t.f$, which we often will do. Restricting to $C_{\mathsf{u}}(G)$, we thus obtain a norm-preserving, and in particular continuous, action of G on $C_{\mathsf{u}}(G)$. It is also continuous with respect to the weak topology. The set $G.f := \{t.f : t \in G\}$ is the *G-orbit* of f. Translation of measures on G works in the same way, $(t.\mu)(f) := \mu(T_t^{-1}f) = \mu(T_{-t}f)$.

The basic idea behind almost periodicity is that a function on G is almost periodic if its translation orbit (or G-orbit) $G.f$ has compact closure. What distinguishes different types of almost periodicity are the classes of functions that we take and the topologies that we use to form the closure of the orbits. We shall always be in the context of uniform topologies, and in these cases

we can replace compactness of the closure of $G.f$ by the total boundedness of $G.f$ itself; compare [8]. This fact will be used frequently in the sequel.

Proposition 4.1.4 ([23]). *A uniform space is totally bounded if and only if each net in the space has a Cauchy subnet.* □

Definition 4.1.5. Let G be an LCAG. A function $f \in C_{\mathsf{u}}(G)$ is *strongly* (respectively *weakly*) *almost periodic* if the closure of $G.f$ in the strong (respectively weak) topology is compact. The spaces of strongly and weakly almost periodic functions on G are denoted by $\mathrm{SAP}(G)$ and $\mathrm{WAP}(G)$, respectively.

It is easy to see that $\mathrm{SAP}(G)$ and $\mathrm{WAP}(G)$ are vector subspaces of $C_{\mathsf{u}}(G)$ and that $\mathrm{SAP}(G) \subseteq \mathrm{WAP}(G)$, the latter via Eq. (4.1.2).

Since the translation operators $T_t \colon C_{\mathsf{u}}(G) \longrightarrow C_{\mathsf{u}}(G)$ are equicontinuous in the strong topology, and $(C_{\mathsf{u}}(G), \|.\|_\infty)$ is a Banach space, the definition of strong almost periodicity for functions is equivalent to both the Bochner and Bohr definitions of almost periodicity.

As observed in [15], the study of weak almost periodicity is more complicated. The translation operators $T_t \colon C_{\mathsf{u}}(G) \longrightarrow C_{\mathsf{u}}(G)$ are weakly continuous but not weakly equicontinuous, and this makes the Bochner and Bohr definitions of almost periodicity different. The matters are complicated further by the fact that $C_{\mathsf{u}}(G)$ is not complete in the weak topology, which means that totally boundedness of the orbit is not enough to guarantee weak almost periodicity.

Ultimately, in Section 4.10, we will study almost periodicity in the space of translation bounded measures on G. The key to the transition from functions to measures is that μ is a translation bounded measure if and only if, for all $f \in C_{\mathsf{c}}(G)$, the convolution satisfies $\mu * f \in C_{\mathsf{u}}(G)$. Then, μ is almost periodic if and only if $\mu * f$ is almost periodic for all $f \in C_{\mathsf{c}}(G)$, and again we shall have weak and strong almost periodicity according to which type of almost periodicity we wish to use.

One of the important tools in the study of almost periodicity is the notion of the mean of a function. To introduce it, we first recall the notion of a *van Hove sequence*; compare also [AO1, Def. 2.9] and [44, p. 145]. The latter is a sequence $\{A_n\}$ of compact Borel subsets of G such that, for every compact set $K \subseteq G$,

$$\lim_{n\to\infty} \frac{\theta_G\big(((K + A_n) \setminus A_n^\circ) \cup ((-K + \overline{G \setminus A_n}) \cap A_n)\big)}{\theta_G(A_n)} \;=\; 0, \tag{4.1.3}$$

where the bar (circle) denotes the closure (interior) of a set. For simplicity, we shall refer to the argument of θ_G in the numerator of Eq. (4.1.3) as $\partial^K(A_n)$, and call this the *K-boundary* of A_n. Note that one can also work

with a sequence of open sets and adjust the definition of the K-boundary accordingly.

In effect, the slightly technical condition of Eq. (4.1.3) states that, for each compact set $K \subseteq G$, the K-boundary of the averaging sequence becomes measurewise negligible relative to the sequence as $n \to \infty$. Note that general van Hove sequences need not be nested. In the material of this section, the van Hove property could be replaced by the more general Følner condition; see Definition 4.5.1 below. However, the van Hove condition is more commonly used in the subject of aperiodic order; compare [AO1, Sec. 2.3.4].

Definition 4.1.6. The *mean* $M(f)$ (relative to a van Hove sequence $\{A_n\}$ of subsets of G) of a function $f \in C_{\mathsf{u}}(G)$ is

$$M(f) \,=\, \lim_{n\to\infty} \frac{\int_{A_n} f(x+t)\,\mathrm{d}\theta_G(t)}{\theta_G(A_n)}, \tag{4.1.4}$$

if the limit exists uniformly for all $x \in G$.

Note that, if uniform convergence were not assumed, the definition of the mean (and of amenability) would depend of the choice of the van Hove sequence; compare Remark 4.5.7 and Example 4.5.8.

Means were introduced by H. Bohr into his theory of almost periodic functions as a way of getting around the loss of period groups when one passes from periodic to almost periodic functions. For example, a periodic function f on the real line, say of period 1, is in effect a function on the compact circle group[3] $\mathbb{T} = \mathbb{R}/\mathbb{Z}$, equipped with Lebesgue measure $\theta_{\mathbb{T}}$. The Fourier analysis then unfolds around the character theory of the group $\mathbb{T}$, with the orthogonality relations $\int_{\mathbb{T}} \overline{\chi}\,\psi\,\mathrm{d}\theta_{\mathbb{T}} = \delta_{\chi,\psi}$ playing a central role in defining the Fourier coefficients of f through $a_f(\chi) = \int_{\mathbb{T}} \overline{\chi}\, f\,\mathrm{d}\theta_{\mathbb{T}}$. More specifically, the characters are of the form $\chi_k(.) = \mathrm{e}^{2\pi\mathrm{i}k(.)}$ with $k \in \mathbb{Z}$, and the integrals can be expressed accordingly.

In the case of almost periodic (but not periodic) functions, the period group does not exist and there is no reduction to a nice compact group. One has the characters $\chi \in \widehat{\mathbb{R}}$, but the expressions $\int_{\mathbb{R}} \overline{\chi(x)}\, f(x)\,\mathrm{d}x$ do not make sense. Bohr's solution is to instead use averages of the form

$$\lim_{n\to\infty} \frac{1}{2n} \int_{-n}^{n} \overline{\chi(x)}\, f(x)\,\mathrm{d}x.$$

These limits have a chance of existing (and do for the large class of weakly almost periodic functions) and, in the periodic case, yield the same values as obtained from integrating over the circle group $\mathbb{T}$. The definition of a mean in Eq. (4.1.4) is the analogue of this for general LCAGs.

[3] As in [AO1], we distinguish the circle group (or 1-torus) $\mathbb{T}$ from the unit circle $\mathbb{S}^1 := \{z \in \mathbb{C} : |z| = 1\}$, and with it additive versus multiplicative notation.

A major part of this chapter consists of building up a theory of almost periodic functions to which we can apply the concept of means. Here, our aim is to always keep the level of generality in proportion to our needs for the theory of aperiodic order. Our approach to almost periodicity follows that of Eberlein (see our references [15, 16, 17]), and is set up in the context of locally convex topological vector spaces. We have to retain this level of generality here because, although the principal example is $C_{\mathsf{u}}(G)$, we also need Eberlein's theory of systems of almost invariant integrals for $\mathrm{WAP}(G)$; see Proposition 4.7.10 below.

It is for this reason that, although the definitions of strong and weak aperiodicity involve only orbits of the form $G.f$, a good deal of effort has to be put into studying their closed *convex hulls* $\mathcal{C}_f$. Means and systems of almost invariant integrals lead unavoidably to entities lying in convex hulls of the form $\mathcal{C}_f$. Fortunately, although the two topologies potentially give rise to different convex hulls, it turns out that strongly closed convex sets are weakly closed (see Corollary 4.4.12 below), so there is only one convex hull to worry about. We shall see that strong and weak almost periodicity are equivalent to the compactness of $\mathcal{C}_f$ in the strong and weak topologies, respectively.

4.2. Topological background

After our general remarks so far, let us take a closer look at LCAGs and their duals, as well as at the important Bohr compactification.

4.2.1. Character theory and Pontryagin duality

Let G be an LCAG. An *algebraic character* of, or on, G is a group homomorphism $\chi\colon G \longrightarrow U(1) = \mathbb{S}^1$, from G into the unit circle. Here, χ is not assumed to be continuous, though of course it always is if G carries the discrete topology. We will denote by $\widehat{G}_{\mathsf{alg}}$ the set of all characters on G. If χ and ψ are two characters of G, so is their product $\chi\psi$, which is defined by

$$\big(\chi\psi\big)(x) \,=\, \chi(x)\psi(x) \quad \text{for all } x \in G.$$

The trivial character 1, whose value everywhere is 1, is the identity element for this multiplication. With inversion defined by $\chi^{-1}(x) = \overline{\chi(x)}$, the set $\widehat{G}_{\mathsf{alg}}$ becomes an Abelian group. This is the *algebraic dual* of G. The set of all continuous characters forms a subgroup $\widehat{G}$ of $\widehat{G}_{\mathsf{alg}}$. Henceforth, the unmodified word *character* will always mean continuous character, and in keeping with this we call $\widehat{G}$ the *dual group* of G.

Definition 4.2.1. Given G, the group of all algebraic characters $\widehat{G}_{\mathsf{alg}}$ is the *algebraic dual* of G, while the group $\widehat{G}$ of continuous characters is called the *dual group* of G.

It is worth noting that $\widehat{G}_{\mathsf{alg}}$ is also a dual group, namely the dual of $G_{\mathtt{d}}$, which is G equipped with the discrete topology.

The dual $\widehat{G}$ of an LCAG G is also a locally compact Abelian group when we give it the *compact-open topology*. This topology arises by requiring that the family of all sets of the form

$$N(K,\varepsilon) := \big\{\chi \in \widehat{G} : |\chi(x) - 1| < \varepsilon \text{ for all } x \in K\big\},$$

where $\varepsilon > 0$ and K is a compact subset of G, is a basis of open sets at the trivial character $1 \in \widehat{G}$.

Example 4.2.2. In the case of $G = \mathbb{R}^d$, each continuous character is of the form $\chi = \chi_a$ for some $a \in \mathbb{R}^d$, where

$$\chi_a(x) := \mathrm{e}^{2\pi \mathrm{i}\, ax}$$

with ax denoting the inner product in $\mathbb{R}^d$. Hence, the dual group of $\mathbb{R}^d$ is isomorphic (as a topological group) to $\mathbb{R}^d$ by means of $a \longleftrightarrow \chi_a$. Note the possible confusion of the additive notation in $\mathbb{R}^d$ and the multiplicative notation for characters: $a + b \longleftrightarrow \chi_{a+b} = \chi_a \chi_b$. ◊

As usual with duality, we have a natural embedding

$$G \hookrightarrow \widehat{\widehat{G}}, \tag{4.2.1}$$

by identifying each element $x \in G$ with a character on $\widehat{G}$ via $x(\chi) := \chi(x)$. We can now summarise Pontryagin's duality theory as follows.

Theorem 4.2.3. *Let G be a locally compact Abelian group.*

(i) *G and $\widehat{\widehat{G}}$ are isomorphic as topological groups via the embedding of Eq.* (4.2.1)*;*

(ii) *G is compact if and only if $\widehat{G}$ is discrete;*

(iii) *G is discrete if and only if $\widehat{G}$ is compact;*

(iv) *Each continuous homomorphism $\alpha\colon G_1 \longrightarrow G_2$ defines a continuous homomorphism $\widehat{\alpha}\colon \widehat{G_2} \longrightarrow \widehat{G_1}$ via*

$$\widehat{\alpha}(\chi)(x) := \chi\big(\alpha(x)\big);$$

(v) *If $\alpha_1\colon G_1 \longrightarrow G_2$ and $\alpha_2\colon G_2 \longrightarrow G_3$ are continuous homomorphisms, one has $\widehat{\alpha_2 \circ \alpha_1} = \widehat{\alpha_1} \circ \widehat{\alpha_2}$.*

(vi) *Under the identification $\widehat{\widehat{G_i}} = G_i$, for $i \in \{1,2\}$, we have $\widehat{\widehat{\alpha}} = \alpha$ in the notation of* (iv)*;*

(vii) *In the notation of* (iv)*,*

(a) *α has dense image in G_2 if and only if $\widehat{\alpha}$ is one-to-one;*

(b) *α is one-to-one if and only if $\widehat{\alpha}$ has dense image in $\widehat{G_1}$.* □

For further details, proofs and examples, we refer to [41] or [38].

4.2.2. The Bohr compactification

Let G be an LCAG and let $\widehat{G}_{\mathtt{d}}$ denote $\widehat{G}$ equipped with the discrete topology. Then, by Pontryagin duality,

$$G_{\mathrm{B}} \;:=\; \widehat{\widehat{G}_{\mathtt{d}}}$$

is the dual of a discrete group, thus compact. We observe that the identity map $\iota\colon\ \widehat{G}_{\mathtt{d}} \longrightarrow \widehat{G}$ is continuous, one-to-one, and has dense image. Hence, the mapping

$$\widehat{\iota}\colon\ G = \widehat{\widehat{G}} \;\hookrightarrow\; \widehat{\widehat{G}_{\mathtt{d}}} = G_{\mathrm{B}}$$

is continuous, one-to-one and has dense image, and we can identify G with a dense subgroup of the compact group G_{B}.

Definition 4.2.4. The group G_{B} is called the *Bohr compactification* of G.

Example 4.2.5 (*Bohr compactification*)**.** If G is compact, $\widehat{G}$ is already discrete, hence $\widehat{G} = \widehat{G}_{\mathtt{d}}$. Consequently, one has $G = G_{\mathrm{B}}$ in this case.

For $G = \mathbb{R}$, one can start with $\widehat{\mathbb{R}}$, which is isomorphic to $\mathbb{R}$ (as a topological group) via $\exp(2\pi \mathrm{i} a(.)) \mapsto a$. Dualising and making the topology discrete results in $\mathbb{R}_{\mathtt{d}}$. Now, $\widehat{\mathbb{R}_{\mathtt{d}}}$ is the group of all continuous characters on $\mathbb{R}_{\mathtt{d}}$. The latter, due to the discreteness of the space, is just the same as the group of *all* characters (the algebraic homomorphisms of $\mathbb{R}$ into $\mathbb{T}$ as mentioned earlier). So, the Bohr compactification $\mathbb{R}_{\mathrm{B}}$ of $\mathbb{R}$ is the group of all characters, as opposed to the group of all continuous characters.

The true vastness of $\mathbb{R}_{\mathrm{B}} = \widehat{\mathbb{R}_{\mathtt{d}}}$ is seen by taking a Hamel basis B of $\mathbb{R}$ (a basis of $\mathbb{R}$ over $\mathbb{Q}$). Then, one has $\mathbb{R}_{\mathrm{B}} \simeq \mathbb{T}^B$ (as topological groups). For the link between the Bohr compactification and almost periodicity, see Theorem 4.3.5 below.

If $G = \mathbb{Z}$, we have $\widehat{\mathbb{Z}} = \mathbb{T}$. We can now view $\widehat{\mathbb{T}}$ as the group of continuous characters on $\mathbb{R}$ which are trivial on $\mathbb{Z}$. The Bohr compactification $\mathbb{Z}_{\mathrm{B}} = \widehat{\mathbb{T}_{\mathtt{d}}}$ is then the group of algebraic characters on $\mathbb{R}$ that are trivial on $\mathbb{Z}$. So, if our Hamel basis of $\mathbb{R}$ is chosen such that $1 \in B$ and if we set $B' := B \setminus \{1\}$, the Bohr compactification of $\mathbb{Z}$ can be identified with $\mathbb{T}^{B'}$. $\lozenge$

We will always feel free to identify G with its image in G_{B} under $\widehat{\iota}$, and hence consider G to be a dense subgroup of G_{B}. The Bohr compactification has the following important universal property.

Proposition 4.2.6. *Any continuous homomorphism $\alpha\colon\ G \longrightarrow H$ of G into a compact Abelian group H can be factored through G_{B} as*

$$G \xrightarrow{\ \widehat{\iota}\ } G_{\mathrm{B}} \xrightarrow{\ \alpha_{\mathrm{B}}\ } H\,,$$

with $\alpha = \alpha_{\mathrm{B}} \circ \widehat{\iota}$. *The Bohr compactification is unique in the sense that if* $j\colon G \longrightarrow J$ *is any compactification of* G, *that is to say,* j *is a continuous injective homomorphism with dense image in the compact Abelian group* J *that satisfies this same universal property, then there is a unique isomorphism* $\beta\colon G_{\mathrm{B}} \longrightarrow J$ *with* $j = \beta \circ \widehat{\iota}$.

Proof. The mapping $\widehat{\alpha}\colon \widehat{H} \longrightarrow \widehat{G}$ factorises through $\widehat{G}_{\mathsf{d}}$ since $\widehat{H}$ is discrete, so $\widehat{H} \longrightarrow \widehat{G}_{\mathsf{d}} \longrightarrow \widehat{G}$. Dualising this gives the desired factorisation of α.

As for the uniqueness, if (J, j) is another pair with the same 'universal' property as $(G_{\mathrm{B}}, \widehat{\iota})$, then there are homomorphisms $\beta\colon G_{\mathrm{B}} \longrightarrow J$ as well as $\gamma\colon J \longrightarrow G_{\mathrm{B}}$ for which $j = \beta \circ \widehat{\iota}$ and $\widehat{\iota} = \gamma \circ j$. Since $\widehat{\iota}$ and j are continuous and injective with dense images, β and γ are seen to be inverses of one another, and β is the required isomorphism. □

4.3. Almost periodic functions

Here, we begin our more detailed analysis of almost periodic functions, in their different flavours, how they are connected, and how positive definite functions fit into the picture.

4.3.1. Characterisations of almost periodicity

Let G be an LCAG. Concerning the notions of $\mathrm{SAP}(G)$ and $\mathrm{WAP}(G)$ from Definition 4.1.5, recall that, for $f \in C_{\mathsf{u}}(G)$, almost periodicity requires compactness of the closure of $G.f$ in the strong or weak topology, respectively.

Example 4.3.1. Since all elements $\chi \in \widehat{G}$ satisfy

$$\bigl\{T_t\chi : t \in G\bigr\} \subseteq \bigl\{a\chi : a \in \mathbb{S}^1\bigr\},$$

where the latter is compact, they are all strongly almost periodic. As $\mathrm{SAP}(G)$ is a vector space, we see that all *trigonometric polynomials* $\sum_{i=1}^{n} a_i\chi_i$, where $\chi_i \in \widehat{G}$ and $a_i \in \mathbb{C}$, are strongly almost periodic as well. ◊

As a first step, we recover Bohr's original definition of (strong) almost periodicity; compare [AO1, Sec. 8.2].

Proposition 4.3.2. *Let* $f \in C_{\mathsf{u}}(G)$. *Then,* $f \in \mathrm{SAP}(G)$ *if and only if, for every* $\varepsilon > 0$, *the set* $P_\varepsilon := \bigl\{t \in G : \|T_t f - f\|_\infty < \varepsilon\bigr\}$ *is relatively dense.*

Proof. For brevity, $\|.\|$ denotes the sup-norm on $C_{\mathsf{u}}(G)$ in this proof, and $B_\varepsilon(g)$ is the open ball of radius-ε around $g \in C_{\mathsf{u}}(G)$.

Recall Proposition 4.1.4 and let $f \in \mathrm{SAP}(G)$. Then, $G.f$ is totally bounded, so if $\varepsilon > 0$ is chosen arbitrarily, there are $t_1, \ldots, t_N \in G$ so that

$$\bigcup_{i=1}^{N} B_\varepsilon(t_i.f) \supseteq G.f.$$

Then, for each $x \in G$, there is a t_i from the above list so that $\|x.f - t_i.f\| < \varepsilon$. This gives $y := x - t_i \in P_\varepsilon$, wherefore we have

$$G \,=\, \{t_1, \ldots, t_N\} + P_\varepsilon ,$$

and P_ε is relatively dense.

Conversely, suppose that all the P_ε are relatively dense. Choose an $\varepsilon > 0$. By the uniform continuity of f, there is an open neighbourhood U of $\{0\}$ in G so that $x - y \in U$ implies $\|f(x) - f(y)\| < \varepsilon/2$. By assumption, there is a compact $K \subseteq G$ for which $K + P_{\varepsilon/2} = G$, and the compactness of K implies that there are $t_1, \ldots, t_N \in G$ so that $\bigcup_i (t_i + U) \supseteq K$.

If $t \in G$ is fixed, one has $t = k + p = t_i + u + p$ for some $k \in K$, $u \in U$, $p \in P_{\varepsilon/2}$ and for some t_i with $1 \leqslant i \leqslant N$. Then,

$$\begin{aligned} \|t.f - t_i.f\| \,&=\, \|(u+p).f - f\| \,\leqslant\, \|(u+p).f - u.f\| + \|u.f - f\| \\ &=\, \|(u.(p.f) - u.f\| + \|u.f - f\| \,=\, \|p.f - f\| + \|u.f - f\| \,<\, \varepsilon . \end{aligned}$$

This shows that the ε-balls around $\{t_1.f, \ldots, t_N.f\}$ cover $G.f$, which establishes that the latter is totally bounded. □

Corollary 4.3.3. *If G is compact, one has* $\mathrm{SAP}(G) = \mathrm{WAP}(G) = C(G)$.

Proof. As $\mathrm{SAP}(G) \subseteq \mathrm{WAP}(G) \subseteq C_{\mathsf{u}}(G) \subseteq C(G)$, it suffices to prove $\mathrm{SAP}(G) = C(G)$. Since G is compact, we have $C(G) = C_{\mathsf{u}}(G)$, and any non-empty subset of G is relatively dense. □

4.3.2. WAP(G) and SAP(G) are closed

Proposition 4.3.4 ([15, Thm. 4.2])**.** *Both* $\mathrm{SAP}(G)$ *and* $\mathrm{WAP}(G)$ *are closed subspaces of $C_{\mathsf{u}}(G)$, in the strong topology of $\|.\|_\infty$.*

Proof. Let $\{f_n\} \subset \mathrm{SAP}(G)$ with $f_n \longrightarrow f \in C_{\mathsf{u}}(G)$ in the strong topology. We shall show that $f \in \mathrm{SAP}(G)$ by verifying the relative denseness condition of Proposition 4.3.2.

Let $\varepsilon > 0$. Then, there is some $n_0 \in \mathbb{N}$ such that $\|f_n - f\|_\infty < \frac{\varepsilon}{3}$ holds for all integers $n > n_0$. Let $n > n_0$ be fixed. Since $f_n \in \mathrm{SAP}(G)$, the set $\{x \in G : \|x.f_n - f_n\|_\infty < \frac{\varepsilon}{3}\}$ is relatively dense. Since

$$\left\{x \in G : \|x.f_n - f_n\|_\infty < \tfrac{\varepsilon}{3}\right\} \,\subseteq\, \left\{x \in G : \|x.f - f\|_\infty < \varepsilon\right\}$$

by a standard 3ε-argument, we can conclude that this last set is also relatively dense, as required.

To prove the statement on weak almost periodicity, let $\{f_n\} \subset \mathrm{WAP}(G)$ with $f_n \longrightarrow f \in C_{\mathsf{u}}(G)$. We wish to show that $f \in \mathrm{WAP}(G)$, i.e., that the closure of $G.f$ is weakly compact. We do this by showing that, for any net $\{x_\ell\}$ in G, $\{x_\ell.f\}$ has a subnet which converges to some $g \in C_{\mathsf{u}}(G)$.

Assume that we have a net $\{x_\ell\}$ in G. The G-orbit of $(f_1, f_2, \dots)$ in $C_{\mathsf{u}}(G)^{\mathbb{N}}$ under the diagonal action of G gives us

$$\overline{G.(f_1, f_2, \dots)} \subseteq \overline{G.f_1} \times \overline{G.f_2} \times \cdots ,$$

which is the product of weakly compact sets, hence weakly compact. Thus, we can find a subnet $\{x_{\ell_\alpha}\}$ so that, simultaneously for all n, the net $\{x_{\ell_\alpha}.f_n\}_\alpha$ converges, say

$$\text{w-}\lim_\alpha \big(x_{\ell_\alpha}.f_n\big) \,=\, g_n.$$

Then, with $\|.\|$ denoting the norm on $C_{\mathsf{u}}(G)'$, the estimate

$$\begin{aligned} \|g_n - g_p\|_\infty \,&=\, \sup_{\substack{\phi \in C_{\mathsf{u}}(G)' \\ \|\phi\|=1}} \big|\phi(g_n - g_p)\big| \,=\, \sup_{\|\phi\|=1} \lim_\alpha \big|\phi(x_{\ell_\alpha}.f_n - x_{\ell_\alpha}.f_p)\big| \\ &\leqslant \sup_{\|\phi\|=1} \|\phi\|\, \|f_n - f_p\|_\infty \,=\, \|f_n - f_p\|_\infty \end{aligned}$$

shows that $\{g_n\}$ is Cauchy in $\big(C_{\mathsf{u}}(G), \|.\|_\infty\big)$, because $\{f_n\}$ is convergent and hence Cauchy.

Let $g := \lim_{n\to\infty} g_n$, $\phi \in C_{\mathsf{u}}(G)'$ and $\varepsilon > 0$. There exists an n_0 so that $\big|\phi(g - g_{n_0})\big| < \varepsilon$ and $\|f - f_{n_0}\|_\infty < \varepsilon/(\|\phi\| + 1)$.

Since $\text{w-}\lim_\alpha(x_{\ell_\alpha}.f_{n_0}) = g_{n_0}$, there exists an α_0 so that, for all $\alpha > \alpha_0$, we have

$$\big|\phi(g_{n_0} - x_{\ell_\alpha}.f_{n_0})\big| \,<\, \varepsilon.$$

By combining this with

$$\big|\phi(x_{\ell_\alpha}.f - x_{\ell_\alpha}.f_{n_0})\big| \,\leqslant\, \|\phi\|\,\|x_{\ell_\alpha}.f - x_{\ell_\alpha}.f_{n_0}\|_\infty \,=\, \|\phi\|\,\|f - f_{n_0}\|_\infty \,<\, \varepsilon,$$

we get

$$\big|\phi(g - x_{\ell_\alpha}.f)\big| \,<\, 3\varepsilon.$$

Since ϕ and ε were chosen arbitrarily, this shows that $g = \text{w-}\lim_\alpha(x_{\ell_\alpha}.f)$, which completes the proof. □

4.3.3. Further properties of SAP(G)

Let us now establish two other characterisations of SAP(G) for an arbitrary LCAG G. We begin by recalling that, in Example 4.3.1, we established that all trigonometric polynomials are in SAP(G) and hence, thanks to Proposition 4.3.4, all of their limits in the strong topology are in SAP(G). We shall see that, in fact, all elements of SAP(G) are such uniform limits.

Let $f \in \text{SAP}(G)$. We can introduce a pseudo-metric on G by defining

$$\mathrm{d}_f(x, y) \,:=\, \|T_x f - T_y f\|_\infty.$$

This is a translation invariant pseudo-metric, and it is easy to see that G with the d_f-topology becomes a topological group. We let $i\colon G \longrightarrow G_f$ be

the completion mapping. By the definition of strong almost periodicity of f, G_f is a compact group.

Since f is uniformly continuous on G in the topology given by d_f, the completion theorem implies the existence of a continuous map $F\colon G_f \longrightarrow \mathbb{C}$ so that $f = F \circ i$. Now, as $i\colon G \longrightarrow G_f$ has dense image, Pontryagin duality ensures that the dual map

$$\widehat{i}\colon \widehat{G_f} \longrightarrow \widehat{G}$$

is continuous and one-to-one. This dual map is simply the restriction of characters on G_f to characters on G.

Observe that G_f is a compact group and that $\widehat{G_f}$ is a group of continuous functions on G_f which separate its points (since $\widehat{\widehat{G_f}}$ is identifiable with G_f) and is invariant under complex conjugation. Moreover, $\widehat{G_f}$ contains the constant function that takes the value 1 everywhere. We may thus apply the Stone–Weierstrass theorem [37] to infer that the $\mathbb{C}$-span of $\widehat{G_f}$ is a dense subspace of $C(G_f)$.

Let $\varepsilon > 0$ be fixed. Then, there exist $a_1, \ldots, a_n \in \mathbb{C}$ and $\chi_1, \ldots, \chi_n \in \widehat{G_f}$ so that

$$\Big\| F - \sum_{j=1}^{n} a_j \chi_j \Big\|_\infty < \varepsilon.$$

Restricting all this to G and retaining the symbols χ_j for the restricted characters, we obtain

$$\Big\| f - \sum_{j=1}^{n} a_j \chi_j \Big\|_\infty < \varepsilon.$$

Theorem 4.3.5. *If $f \in C_{\mathsf{u}}(G)$, the following properties are equivalent.*

(i) *One has $f \in \mathrm{SAP}(G)$;*

(ii) *For all $\varepsilon > 0$, the set P_ε of ε-almost periods is relatively dense;*

(iii) *There exists a unique function $f_{\mathrm{B}} \in C(G_{\mathrm{B}})$ so that $f = f_{\mathrm{B}}|_G$;*

(iv) *The function f is the $\|.\|_\infty$-limit of a sequence of trigonometric polynomials.*

The Bohr mapping $(.)_{\mathrm{B}}\colon \mathrm{SAP}(G) \longrightarrow C(G_{\mathrm{B}})$, which is defined by $f \mapsto f_{\mathrm{B}}$, is a G-invariant isometric homeomorphism of $\mathrm{SAP}(G)$ and $C(G_{\mathrm{B}})$, both spaces being given the sup-norm topology.

Proof. We already proved the equivalence of (i), (ii) and (iv). We need to see how the Bohr compactification comes in. First, (iii) $\Longrightarrow$ (iv) is proved just as we did above, with G_{B} replacing G_f.

To finish the equivalences, we now prove (i) $\Longrightarrow$ (iii). Given a function $f \in \mathrm{SAP}(G)$, we need to find an extension of f to G_{B}. Since G embeds densely in G_{B}, the extension will be unique if it exists. Create the compact group G_f

as above. From the continuous map $G \longrightarrow G_f$, the compactness of G_f, and the universal property from Proposition 4.2.6, we have the factorisation

$$G \longrightarrow G_{\mathrm{B}} \longrightarrow G_f, \tag{4.3.1}$$

with the composition of the two maps being i.

We saw that f lifts to a function F on G_f which satisfies $f = F \circ i$. Using Eq. (4.3.1), we pull this back to a continuous function f_{B} on G_{B}, and this map restricts to the original f on G. This is the mapping we are looking for, and this proves (iii).

It is immediate that $\|f_{\mathrm{B}}\|_\infty = \|F\|_\infty = \|f\|_\infty$, so the mapping $(.)_{\mathrm{B}}$ is a homeomorphism. Identifying G with its images in G_f and G_{B}, we find that, for all $x, y \in G$, one has

$$\bigl(y.f_{\mathrm{B}}\bigr)(x) \,=\, \bigl(y.F\bigr)(x) \,=\, F(-y+x) \,=\, f(-y+x) \,=\, \bigl(y.f\bigr)(x),$$

from which we get the G-invariance by the denseness of G in G_{B}. □

We note that, at this point, we have proved the first three statements in the list of Bohr's results, and this even in the setting of general LCAGs.

Corollary 4.3.6. *The space* $\mathrm{SAP}(G)$ *has the following properties.*

(i) $\mathrm{SAP}(G)$ *is a closed linear space;*
(ii) *If* $f \in \mathrm{SAP}(G)$ *and* $t \in G$, *one has* $T_t f \in \mathrm{SAP}(G)$*;*
(iii) $1 \in \mathrm{SAP}(G)$*;*
(iv) *If* $f \in \mathrm{SAP}(G)$, *one also has* $\widetilde{f}, \overline{f}, f^\dagger, |f| \in \mathrm{SAP}(G)$*;*
(v) *If* $f, g \in \mathrm{SAP}(G)$, *one has* $fg \in \mathrm{SAP}(G)$.

Proof. Claim (i) has been proved above, while (ii) and (iii) are clear from the definition of $\mathrm{SAP}(G)$. For (iv) and (v), we use the Bohr mapping and Theorem 4.3.5. In $C(G_{\mathrm{B}})$, these properties are clear. □

4.3.4. Positive definite functions

The objective of this section is to introduce positive definite functions on an LCAG G and to show that the continuous positive definite functions are all in $\mathrm{WAP}(G)$. For further material on this important class of functions, we refer the reader to [5, 41].

Definition 4.3.7. A function $f\colon G \longrightarrow \mathbb{C}$ is called *positive definite* if, for all integers $n > 0$ and for all choices of $a_1, \ldots, a_n \in \mathbb{C}$, the inequality

$$\sum_{i,j=1}^{n} a_i \, f(t_i - t_j) \, \overline{a_j} \;\geqslant\; 0$$

holds for all $t_1, \ldots, t_n \in G$.

Later, we shall always deal with *continuous* positive definite functions f on G. If f is positive definite, $f(0)$ is real and, for all $x \in G$, satisfies $|f(x)| \leqslant f(0)$. In particular, f is bounded. Furthermore, Krein's inequality states that, for any positive definite f and for all $x, y \in G$, one has

$$\big|f(x) - f(y)\big|^2 \leqslant 2f(0)\big(f(0) - \mathrm{Re}(f(x-y))\big); \tag{4.3.2}$$

see [5, §3.3] for details. An important consequence of Krein's inequality is that any continuous, positive definite function f is actually uniformly continuous, so $f \in C_{\mathsf{u}}(G)$.

One way to obtain positive definite functions is to take an inner product space[4] $\big(H, \langle\cdot|\cdot\rangle\big)$ on which G acts continuously as a group of isometries, choose a $d \in H$, and define $f\colon G \longrightarrow \mathbb{C}$ by

$$t \longmapsto f(t) := \langle d | t.d \rangle. \tag{4.3.3}$$

Just remember that our group is written additively, so that, for isometries $s, t \in G$, one has $\langle d|(s-t).d\rangle = \langle t.d|s.d\rangle$. Therefore, for all $a_1, \ldots, a_n \in \mathbb{C}$ and for all $t_1, \ldots, t_n \in G$, we have

$$\sum_{i,j=1}^{n} a_i\, f(t_i - t_j)\, \overline{a_j} \;=\; \left\langle \sum_{j=1}^{n} a_j t_j.d \,\middle|\, \sum_{i=1}^{n} a_i t_i.d \right\rangle \;\geqslant\; 0.$$

Consequently, all f defined by Eq. (4.3.3) are positive definite.

Let us next show that all positive definite functions arise in this way. To see this, let $f\colon G \longrightarrow \mathbb{C}$ be positive definite and define $\mathcal{F}(G)$ to be the set of all pure point measures μ on G which are supported on only *finitely* many points of G. Define $\phi_f\colon \mathcal{F}(G) \longrightarrow \mathbb{C}$ by

$$\phi_f(\mu) \;=\; \mu(f) \;=\; \sum_{x \in G} f(x) \mu\big(\{x\}\big),$$

and define $\langle\cdot|\cdot\rangle\colon \mathcal{F}(G) \times \mathcal{F}(G) \longrightarrow \mathbb{C}$ via

$$\langle \mu | \nu \rangle \;:=\; \phi_f(\widetilde{\mu} * \nu).$$

Recall that the tilde operation on measures is defined by $\widetilde{\nu}(g) = \overline{\nu(\widetilde{g})}$. Consequently, one has

$$\widetilde{\mu} * \nu \;=\; \sum_{\substack{x \in S_\mu \\ y \in S_\nu}} \overline{\mu(\{x\})}\, \nu(\{y\})\, \delta_{y-x},$$

where $S_\mu = \{z \in G : \mu(\{z\}) \neq 0\}$ and $S_\nu = \{z \in G : \nu(\{z\}) \neq 0\}$ are the finite supports of the measures μ and ν. For the more general convolution of measures, see Definition 4.9.18 below; compare also [AO1, Sec. 8.6].

[4]Note that we use the convention where the inner product $\langle\cdot|\cdot\rangle$ is linear in the second and semi-linear in the first argument.

One checks immediately from the definitions that $\langle\cdot|\cdot\rangle$ is G-invariant and that $\langle\mu|\mu\rangle \geqslant 0$ for all such measures μ, so $\langle\cdot|\cdot\rangle$ is a positive Hermitian form. It induces an obvious uniformity on $\mathcal{F}(G)$, and the Hausdorff completion H of this construction is a Hilbert space. We continue to use the notation $\langle\cdot|\cdot\rangle$ for the inner product. Note that the completion step also kills off all null vectors of $\langle\cdot|\cdot\rangle$ in $\mathcal{F}(G)$.

Let d denote the image of the measure $\delta_0 \in \mathcal{F}(G)$ in H. A short calculation gives

$$\langle d|t.d\rangle \,=\, \phi_f\big(\widetilde{\delta_0} * \delta_t\big) \,=\, f(t),$$

which shows that we have the desired Hilbert space representation of f.

Proposition 4.3.8 ([15, Thm. 11.2])**.** *If f is a continuous and positive definite function on G, then $f \in \mathrm{WAP}(G)$.*

Proof. The proof uses ideas that are reviewed below in Section 4.4.1. Write f in the form of Eq. (4.3.3) for some Hilbert space $\big(H, \langle\cdot|\cdot\rangle\big)$ on which the elements of G act as isometries, and let $d \in H$. Let $\|.\|$ denote the corresponding norm on H. We define $F\colon H \longrightarrow C_{\mathsf{u}}(G)$ by

$$F(h)(t) \,=\, \langle d|t.h\rangle.$$

We first show that F is a continuous mapping of the Banach space H into the Banach space $C_{\mathsf{u}}(G)$. This follows from

$$|F(h)(t)| \,\leqslant\, \|t.h\|\|d\| \,=\, \|h\|\|d\|,$$

and thus

$$\|F\| \,\leqslant\, \|d\|.$$

Next, consider the ball $B := \{k : \|k\| \leqslant \|d\|\}$ in H. Since H is self-dual, it can be identified with H', and B can be viewed as the ball of radius $\|d\|$ in H'. Then, by Theorem 4.4.6 (Banach–Alaoglu), B is weak-$*$ compact in H'. When we identify H with H', the weak topology on H coincides with the weak-$*$ topology on H'. Consequently, B is weakly compact in H. Since F is strongly continuous, one finds that it is also weakly continuous, see Lemma 4.4.2 below, and it follows that $F(B)$ is then weakly compact in $C_{\mathsf{u}}(G)$.

Now, we have our function f with $f(t) = \langle d|t.d\rangle$. For any $u \in G$, we see that the continuous action of G via $u.f$ satisfies

$$\big(u.f\big)(t) \,=\, \big\langle d|(t-u).d\big\rangle \,=\, \big\langle d|t.((-u).d)\big\rangle \,=\, F\big((-u).d\big)(t).$$

Since $\|(-u).d\| = \|d\|$, we thus have $u.f \in F(B)$ and hence $G.f \subseteq F(B)$, from which it follows that the weak closure of $G.f$ is weakly compact. This shows that $f \in \mathrm{WAP}(G)$. □

Remark 4.3.9. It is easy to see that analogously we can prove the following result, which is relevant to Section 4.4.1 below (see the definitions there).

Let E be a locally convex topological vector space with a continuous action of G on it, and let E' be its dual. We will denote by $\langle x, y\rangle$ the dual pairing of the elements $x \in E$ and $y \in E'$. We can define a natural group action of G on E' via

$$\langle x, t.y\rangle \,=\, \langle t.x, y\rangle .$$

It is straightforward to see that this action is continuous with respect to the weak topology on E'.

Now, let us fix $x \in E$ and $y \in E'$. If the closure of $\{t.y\}_{t\in G}$ is weakly compact in E', then the function

$$f(t) \,:=\, \langle x, t.y\rangle$$

is weakly almost periodic in G. Moreover, if $E'' = E$, where E'' denotes the bi-dual (or second dual) of E, the closure of $\{t.y\}_{t\in G}$ is weakly compact by Theorem 4.4.6 (Banach–Alaoglu). ♢

Next, let $1 < p, q < \infty$ with $\frac{1}{p} + \frac{1}{q} = 1$. Then, we have $\bigl(L^p(G)\bigr)' = L^q(G)$ and $\bigl(L^q(G)\bigr)' = L^p(G)$. Moreover, for all $f \in L^p(G)$ and $g \in L^q(G)$, we have

$$\bigl(f * g\bigr)(t) \,=\, \langle f, t.\widetilde{g}\,\rangle \,=\, \int_G f(z)\, g(t-z)\, \mathrm{d}z.$$

Setting $E = L^p(G)$, we have $E' = L^q(G)$ together with $E'' = E$. Therefore, Remark 4.3.9 has the following consequence.

Proposition 4.3.10 ([15, Cor. 11.3.1])**.** *If $f \in L^p(G)$ and $g \in L^q(G)$ with $1 < p, q < \infty$ and $\frac{1}{p} + \frac{1}{q} = 1$, one has $f * g \in \mathrm{WAP}(G)$.* □

We assemble fundamental results about $\mathrm{WAP}(G)$ as follows.

Proposition 4.3.11 ([15, Thm 11.2])**.** *The space $\mathrm{WAP}(G)$ has the following properties.*

(i) $\mathrm{WAP}(G)$ *is a closed linear space;*
(ii) *If $f \in \mathrm{WAP}(G)$ and $t \in G$, then $T_t f \in \mathrm{WAP}(G)$;*
(iii) $1 \in \mathrm{WAP}(G)$*;*
(iv) *If $f \in \mathrm{WAP}(G)$, one also has $\widetilde{f}, \overline{f}, f^{\dagger} \in \mathrm{WAP}(G)$;*
(v) *If $f, g \in \mathrm{WAP}(G)$, then $fg \in \mathrm{WAP}(G)$;*
(vi) *If $f \in \mathrm{WAP}(G)$ and $p > 0$, then $|f|^p \in \mathrm{WAP}(G)$.*

Of these statements, the first four are clear from the definitions and from what we have proved so far. We delay the proof of the last two claims to Section 4.4.5, where we provide more background from the theory of linear operators on Banach spaces.

4.4. Weak topologies and consequences

In dealing with weakly almost periodic functions, we are involved with compactness in weak topologies. There are several issues that arise around this. The first is that compactness and sequential compactness are not necessarily the same thing in this context. WAP is defined in terms of weak compactness, but, from a technical point of view, sequential compactness is what we need. The second issue is that we have to deal with closed convex hulls of weakly compact sets and we will need to prove that they are compact, too. At the outset, none of this is clear. In this section, we deal with these questions. The key results are the Mazur–Bourgin theorem, the Eberlein–Šmulian theorem, and the Krein–Šmulian theorem. A useful source of background for this material is [36].

4.4.1. Locally convex topological vector spaces

There are various equivalent definitions of locally convex topological vector spaces (LCTVS). Following [37], we shall define them as complex vector spaces whose topology is generated by a family of semi-norms that separate the points of the space. In particular, LCTVSs are Hausdorff spaces. Every Banach space (complete normed vector space) is an LCTVS. Given a locally convex topological vector space E, we let E' be the space of all continuous linear functionals on E (the dual space of E), where $\mathbb{C}$ is equipped with its usual (metric) topology to define the continuity of the functionals.

The most important example of E for our purposes is the Banach space $C_{\mathsf{u}}(G)$ for an LCAG G, with the topology given by the sup-norm. For this reason, we shall often denote elements of E by letters like f or g. Note that E can be equipped with various different topologies (beyond its norm topology). Just as for $C_{\mathsf{u}}(G)$, we thus introduce a weak topology on E as well.

Definition 4.4.1. The *weak topology* on an LCTVS E is the weakest topology that makes all linear functionals $\phi \in E'$ continuous.

Thus a net $\{f_\alpha\} \subset E$ converges in the weak topology to an element f if and only if $\phi(f_\alpha) \longrightarrow \phi(f)$ for all $\phi \in E'$. The weak topology is then defined by the family of semi-norms $\|.\|_\phi$; compare Definition 4.1.3. By construction, E with the weak topology is also an LCTVS.

If $\phi_1, \ldots, \phi_n \in E'$ and $\varepsilon > 0$, the set

$$U[\phi_1, \ldots, \phi_n; \varepsilon] := \{x \in E : |\phi_i(x)| < \varepsilon,\, 1 \leqslant i \leqslant n\} \tag{4.4.1}$$

is called a *cylinder set*. The set of all cylinder sets forms a basis of open sets at 0 for the weak topology on E, from which the entire topology is defined. This is also true if we take only those cylinder sets in which $\phi_1, \ldots, \phi_n$ are linearly independent.

We will refer to the original topology on E as the *strong* topology. From the definitions, it is clear that the identity mapping

$$\mathrm{id}\colon E_{\mathrm{strong}} \longrightarrow E_{\mathrm{weak}} \tag{4.4.2}$$

is continuous [37, p. 112]. Much of Section 4.4 is devoted to studying the relationships between strong and weak topologies, which play a crucial role in the theory of almost periodic measures. Topological properties (such as 'closed') will be preceded by the word *weak* when we mean the weak topology; otherwise they should be assumed to pertain to the strong topology.

It follows from Eq. (4.4.2) that, if $M \subseteq E$ is weakly closed, then it is strongly closed, and if M is strongly compact, then it is weakly compact.

Lemma 4.4.2. *If B and C are Banach spaces and $T : B \longrightarrow C$ is a continuous linear mapping, then T is also continuous in the weak topologies.*

Proof. It suffices to show continuity at the origin, and for this it suffices to show that the inverse image under T of every cylinder set of C of the form (4.4.1) is a cylinder set of B. But this is clear, because one can verify that

$$T^{-1}\big(U[\phi_1, \phi_2, \ldots, \phi_n; \varepsilon]\big) \;=\; U[\psi_1, \psi_2, \ldots, \psi_n; \varepsilon],$$

where the functionals $\psi_i := \phi_i \circ T$ are continuous by the continuity of T. □

One of the fundamental theorems of functional analysis is the Hahn–Banach theorem (see, for example, [24, 53]). We state it here in a version that covers both its real and its complex form.

Theorem 4.4.3 (Hahn–Banach)**.** *Let E be a linear space over $\mathbb{R}$. Suppose that $p\colon E \longrightarrow \mathbb{R}$ satisfies the conditions*

(i) $p(ax) = a\,p(x)$,

(ii) $p(x + y) \leqslant p(x) + p(y)$,

for all $x, y \in E$ and all $a \geqslant 0$. Let F be a linear subspace of E and let ϕ be any linear functional on F that is dominated by p,

$$\phi(x) \;\leqslant\; p(x) \quad \textit{for all } x \in F.$$

Then, ϕ can be extended to a real-valued linear functional on E that is dominated by p on all of E.

Likewise, let E be a linear space over $\mathbb{C}$ and let $p\colon E \longrightarrow \mathbb{R}$ satisfy

(i) $p(ax) = |a|\,p(x)$,

(ii) $p(x + y) \leqslant p(x) + p(y)$,

for all $a \in \mathbb{C}$ and all $x, y \in E$. If F is a linear subspace of E and ϕ a linear functional on F that is dominated by p, here as

$$|\phi(x)| \;\leqslant\; p(x) \quad \textit{for all } x \in F,$$

the functional ϕ can be extended to a linear functional on E that is dominated by p on all of E. □

A simple application of the Hahn–Banach theorem gives the following useful fact.

Lemma 4.4.4. *Let $(E, \|.\|)$ be a Banach space, and let F be a closed subspace of E. Then, the weak topology on $(F, \|.\|)$ coincides with the induced weak topology as a subset of E.*

PROOF. We need to show that, for any net $\{x_\alpha\} \subset F$ and $x \in F$, we have

$$\{x_\alpha\} \xrightarrow{\text{weakly in } F} x \quad \Longleftrightarrow \quad \{x_\alpha\} \xrightarrow{\text{weakly in } E} x.$$

$\Longrightarrow$: Let $\phi \in E'$. Since $F \subseteq E$, the restriction satisfies $\phi|_F \in F'$. Now, since $\{x_\alpha\} \xrightarrow{\text{weakly in } F} x$, we have $\{\phi|_F(x_\alpha)\} \longrightarrow \phi|_F(x)$ and therefore also $\{\phi(x_\alpha)\} \longrightarrow \phi(x)$. This shows that $\{\phi(x_\alpha)\} \longrightarrow \phi(x)$ for all $\phi \in E'$.

$\Longleftarrow$: Let $\phi \in F'$. By the Hahn–Banach theorem, there exists some $\psi \in E'$ such that $\phi = \psi|_F$. Since $\{x_\alpha\} \xrightarrow{\text{weakly in } E} x$, we have $\{\psi(x_\alpha)\} \longrightarrow \psi(x)$, which implies $\{\phi(x_\alpha)\} \longrightarrow \phi(x)$. This shows that $\{\phi(x_\alpha)\} \longrightarrow \phi(x)$ for all functionals $\phi \in F'$. □

As a consequence, when we have a closed subspace F of a Banach space E, we can speak about weak convergence in F without having to specify whether we mean weak convergence in $(E, \|.\|)$ or weak convergence in $(F, \|.\|)$.

The dual E' of a Banach space E is itself a Banach space with the norm

$$\|\phi\| := \sup_{\substack{x \in E \\ \|x\|=1}} |\phi(x)|.$$

Since E' is a Banach space, so is its dual E''. There is a natural embedding

$$J\colon E \hookrightarrow E'', \tag{4.4.3}$$

since every element x of E can be viewed as a continuous linear functional on E' through $\phi \mapsto \phi(x)$. This mapping is norm preserving and one can view E as a normed subspace of E''.

Along with the weak topology on E, we have the weak-$*$ topology on E'. This is the weakest topology on E' for which all the linear functionals on E' defined by $\phi \mapsto \phi(x)$, where $x \in E$, are continuous.

Since E' is a Banach space, it has its own weak topology, which is defined as the weakest topology on E' for which all the elements of E'' are continuous. This topology is stronger than the weak-$*$ topology (that is, weak-$*$ open sets are weakly open sets, but not necessarily vice versa).

A result that combines some of these ideas is Goldstine's theorem, which we will use later on.

Theorem 4.4.5 (Goldstine). *If E is a Banach space and B is the closed unit ball (in the norm topology) of E, then $J(B)$ is weak-$*$ dense in the unit ball B'' of E''.*

PROOF.[5] The weak-$*$ topology of E'' is defined through the elements of E'. With this in mind, we show that for any $x'' \in B''$, any $\delta > 0$, and any linearly independent set of functionals $\phi_1, \ldots, \phi_n \in E'$, there is a $y \in B$ satisfying

$$x'' - J(y) \in U[\phi_1, \ldots, \phi_n; \delta].$$

In fact, we show that there is an $x \in (1+\delta)B$ so that $\phi_i(x) = x''(\phi_i)$ for all $1 \leqslant i \leqslant n$, so $y := \frac{x}{1+\delta}$ will do the job.

To this end, consider the surjective linear mapping $E \longrightarrow \mathbb{C}^n$ that is defined by $x \mapsto (\phi_1(x), \ldots, \phi_n(x))$, and let its kernel be K. Since the ϕ_i are linearly independent, we can find an $x \in E$ that satisfies $\phi_i(x) = x''(\phi_i)$ for all $1 \leqslant i \leqslant n$, and then all elements of the coset $x + K$ also satisfy the same equations. So, we only need to show that $(x + K) \cap (1 + \delta)B \neq \varnothing$.

If $(x + K) \cap (1 + \delta)B$ were empty, then $\inf\{\|x - k\| : k \in K\} > 1 + \delta$, and so, by Theorem 4.4.3 (Hahn–Banach), we can find a $\phi \in E'$ so that $\phi(K) = \{0\}$ and $\phi(x) > 1 + \delta$. In particular, ϕ factors through K and so is in the linear span of $\{\phi_1, \ldots, \phi_n\}$. Thus, $x''(\phi) = \phi(x) > 1 + \delta$, contrary to $\|x''\| \leqslant 1$. □

An important theorem that we will use a number of times is the well-known Banach–Alaoglu theorem.

Theorem 4.4.6 (Banach–Alaoglu [37]). *Let E be a Banach space. Then, the closed unit ball $B = \{\phi \in E' : \|\phi\| \leqslant 1\}$ of E' is weak-$*$ compact. Likewise, the closed subset $\{\phi \in E' : \|\phi\| = 1\}$ is weak-$*$ compact as well.* □

In the remainder of this section, the notion of boundedness will play an important role. We start by recalling its definition.

Definition 4.4.7. A subset A of a normed vector space $(E, \|.\|)$ is called *bounded* if there exists some constant C such that $\|a\| \leqslant C$ holds for all $a \in A$. It is called *weakly bounded* in E if, for all $\phi \in E'$, the set $\{\phi(a) : a \in A\}$ is bounded in $\mathbb{C}$.

One of the most useful tools for the study of boundedness is the *uniform boundedness principle*.

Theorem 4.4.8 (Uniform Boundedness Principle). *Let E be a Banach space, N a normed space, and let $T_\alpha : E \longrightarrow N$ with $\alpha \in I$ be continuous linear operators. If, for each $x \in E$, the set $\{T_\alpha(x)\}_{\alpha \in I}$ is bounded, the set $\{\|T_\alpha\|\}_{\alpha \in I}$ is bounded as well.* □

[5] This proof derives from a Wikipedia article on Goldstine's theorem.

For a proof of the uniform boundedness principle, which is also known as the Banach–Steinhaus principle, we refer the reader to [13, Sec. II.3]; see also [53].

It is easy to see that every bounded set is weakly bounded. One of the important properties of the weak topology is the fact that each weakly bounded set is bounded.

Lemma 4.4.9. *Let $E \neq \{0\}$ be a Banach space, and let $A \subset E$. Then, A is bounded if and only if A is weakly bounded.*

Proof.
$\Longrightarrow$: When A is bounded, there exists some C such that $\|a\| \leqslant C$ for all $a \in A$. Now, if $\phi \in E'$, the set $\{\phi(a) : a \in A\}$ is bounded by $C\|\phi\|$.
$\Longleftarrow$: Each $a \in A$ defines a linear operator

$$D_a \colon E' \longrightarrow \mathbb{C}, \quad D_a(\phi) = \phi(a).$$

Since A is weakly bounded, the set $\{D_a(\phi)\}_{a\in A}$ is bounded for each $\phi \in E'$. Therefore, by the uniform boundedness principle, the set

$$\big\{\|D_a\| : a \in A\big\}$$

is bounded in the norm topology of E''. Next, by Theorem 4.4.3 (Hahn–Banach), we have $\|D_a\| = |a|$ for all $a \in A$. □

4.4.2. The Mazur–Bourgin theorem

Let E be an LCTVS and consider a semigroup $\mathcal{R}$ of continuous linear operators on E. Then, employing convex combinations, we define the set of mappings

$$\mathcal{R}^* := \big\{r^* = \textstyle\sum_i a_i R_i : a_i \geqslant 0, \sum_i a_i = 1, R_i \in \mathcal{R}\big\}, \tag{4.4.4}$$

where all sums are *finite*. Then, the set $\mathcal{R}^*$ is also a semigroup under composition. For an element $f \in E$, we define

$$\begin{aligned} \mathcal{R}f &= \{Rf : R \in \mathcal{R}\}; \\ O_f &= O_f(\mathcal{R}) := \mathcal{R}^* f = \{r^* f : r^* \in \mathcal{R}^*\}; \\ \mathcal{C}_f &= \mathcal{C}_f(\mathcal{R}) := \overline{O_f(\mathcal{R})}. \end{aligned} \tag{4.4.5}$$

The necessity of studying convex sets like $\mathcal{C}_f$ lies in the development of one of the main tools to study WAP, namely the mean $M(f)$ of a function, which by construction involves limits of convex combinations of translates of the function. The mean itself derives from systems of almost invariant integrals, see Definition 4.4.33, which again involve convex sets like $\mathcal{C}_f$.

Clearly, O_f is the convex hull of $\mathcal{R}f$, and $\mathcal{C}_f$ is its closure. The closure here is in the strong topology, but the main point of this section is to prove

the Mazur–Bourgin theorem which states that it makes no difference whether we take the strong or the weak closure.

The normal situation for us is $E = C_{\mathsf{u}}(G)$, and we shall most often take $\mathcal{R} = \{T_x : x \in G\}$, which is even a *group* of continuous linear operators on $C_{\mathsf{u}}(G)$. In this case, $\mathcal{C}_f$ is the closed convex hull in $C_{\mathsf{u}}(G)$ of the orbit $G.f$. We shall often write $\mathcal{G}^*$ for $\mathcal{R}^*$ in this case. However, one of the important applications of semigroups of operators will occur in the decomposition of the space $\mathrm{WAP}(G)$, where a very different semigroup of operators will appear; see Theorem 4.7.10.

Theorem 4.4.10 (Mazur–Bourgin [10, 34, 43])**.** *In any LCTVS, closed convex sets are weakly closed.*

Before we prove this theorem, let us discuss its relevance. We will use it several times in the sequel. The first use will appear in the following form.

Corollary 4.4.11. *In any LCTVS, closed subspaces are weakly closed.* □

We remark in passing that, if E is a Banach space, as it will be in most of the cases in which we use this result, Corollary 4.4.11 is also an immediate consequence of Theorem 4.4.3 (Hahn–Banach). Indeed, if F is a closed subspace of E and $x \notin F$, then the Hahn–Banach theorem implies the existence of some $\phi \in E'$ such that $\phi(x) = \|x\|$ and $\phi(y) = 0$ for all $y \in F$. Consequently, x cannot be a weak cluster point of F.

The second important consequence is the following, which derives from the Mazur–Bourgin theorem and the fact that weakly closed always implies strongly closed.

Corollary 4.4.12. *Let G be an LCAG and R a representation of G by continuous operators on an LCTVS E. Then, for all $f \in E$, the set $\mathcal{C}_f$ is both the strong and the weak closure of O_f.* □

As we shall see below, Theorem 4.4.10 is a consequence of the Hahn–Banach theorem in conjunction with properties of the Minkowski functional for convex sets. We start by reviewing some basic results of convex analysis; for a more detailed review, see [43, Ch. 3].

Definition 4.4.13. Let E be an LCTVS and let K be a convex subset of E so that 0 is an interior point of K. We define the *Minkowski functional* of K as the mapping $p_K \colon E \longrightarrow [0, \infty)$ with

$$p_K(x) = \inf\bigl\{t \in \mathbb{R}_+ : x \in tK\bigr\}.$$

Proposition 4.4.14. *For each convex neighbourhood K of 0, the Minkowski functional p_K satisfies the following properties,*

(i) $p_K(x) \geqslant 0$ *for all* $x \in E$;

(ii) $p_K(x) < \infty$ *for all* $x \in E$;
(iii) $p_K(x) \leqslant 1$ *for all* $x \in K$;
(iv) $p_K(ax) = ap_K(x)$ *for all* $x \in E$ *and for all* $a \geqslant 0$;
(v) $p_K(x+y) \leqslant p_K(x) + p_K(y)$ *for all* $x, y \in E$;
(vi) $K^\circ = \{x \in E : p_K(x) < 1\}$.

PROOF. Claims (i)–(iv) are clear.

To establish (v), let $p_K(x) = s$, $p_K(y) = t$, and choose an $\varepsilon > 0$. Then, $x \in (s+\varepsilon)K$ and $y \in (t+\varepsilon)K$. Thus, there exist $k_1, k_2 \in K$ so that $x = (s+\varepsilon)k_1$ and $y = (t+\varepsilon)k_2$. By the convexity of K,

$$k := \frac{s+\varepsilon}{s+t+2\varepsilon}\, k_1 + \frac{t+\varepsilon}{s+t+2\varepsilon}\, k_2 \in K,$$

and

$$x + y = (s+\varepsilon)k_1 + (t+\varepsilon)k_2 = (s+t+2\varepsilon)k.$$

Thus, $p_K(x+y) \leqslant p_K(x) + p_K(y) + 2\varepsilon$, and this is true for all $\varepsilon > 0$.

For (vi), we establish the equality by double inclusion. On the one hand, $x \in K^\circ$ means that there exists an $\varepsilon > 0$ so that $x + \varepsilon x \in K$. Thus, $x \in \frac{1}{1+\varepsilon}K$, and $p_K(x) < 1$.

On the other hand, $p_K(x) < 1$ implies $x \in K$ since K is convex and $0 \in K$. Let ε be chosen so that $0 < \varepsilon < 1 - p_K(x)$. Then, for all $y \in K$,

$$p_K(x + \varepsilon y) \leqslant p_K(x) + \varepsilon p_K(y) < 1,$$

and we conclude that $x + \varepsilon K \subset K$, so $x \in K^\circ$. □

Proposition 4.4.15. *Let E be a real LCTVS, and let M and N be nonempty convex subsets, with M open and $M \cap N = \varnothing$. Then, there exists a continuous linear functional $0 \neq f\colon E \longrightarrow \mathbb{R}$ so that, for all $x \in M$ and all $y \in N$, we have $f(x) \leqslant f(y)$.*

PROOF. Pick a p so that $-p \in \operatorname{int}(M - N)$ and define $K := M - N + p$. Then, K is convex and 0 is an interior point of K. Let p_K be the Minkowski functional of K. Since $p \notin K$, we have $p_K(p) \geqslant 1$.

Define the linear functional g on $\mathbb{R}p$ by

$$g(ap) := ap_K(p).$$

Then, one has

$$g(ap) = p_K(ap), \quad \text{for all } a \geqslant 0;$$
$$g(ap) < p_K(ap), \quad \text{for all } a < 0.$$

Using the Hahn–Banach theorem (see Theorem 4.4.3, real case) and the fact that p_K satisfies Proposition 4.4.14(iv) and (v), there exists a linear functional

$f\colon E \longrightarrow \mathbb{R}$ which extends g and satisfies

$$f(x) \leqslant p_K(x) \quad \text{for all } x \in E.$$

Let $x \in M$ and $y \in N$. Then, $x - y + p \in K$ and hence

$$f(x) - f(y) + f(p) = f(x - y + p) \leqslant p_K(x - y + p) \leqslant 1 \leqslant g(p) = f(p),$$

so $f(x) \leqslant f(y)$, which we wished to show. Also, since $f(x) \leqslant 1$ on the open set $K^\circ \neq \varnothing$, f is continuous. This establishes the existence of the required functional f. □

Proposition 4.4.16. *Let E be a complex LCTVS, and let N be a closed convex subset. If $x \notin N$, there exists a continuous functional $g\colon E \longrightarrow \mathbb{C}$ and some $\delta > 0$ so that, for all $y \in N$, we have*

$$\operatorname{Re}\bigl(g(x)\bigr) + \delta \leqslant \operatorname{Re}\bigl(g(y)\bigr).$$

Proof. Since N is closed and $x \notin N$, there exists a convex open neighbourhood M of x so that $M \cap N = \varnothing$.

Since E is a complex LCTVS, it is also a real LCTVS. Let f be a real linear functional according to Proposition 4.4.15, so $f(z) \leqslant f(y)$ for all $z \in M$ and $y \in N$. Then, $g\colon E \longrightarrow \mathbb{C}$ defined by $g(u) := f(u) - \mathrm{i}f(\mathrm{i}u)$ is complex linear with $\operatorname{Re}(g) = f$.

Since $f \neq 0$, there exists an $x_0 \in E$ so that $f(x_0) = 1$. Let δ be so that $x + \delta x_0 \in M$. Then, for all $y \in N$,

$$f(x) + \delta = f(x + \delta x_0) \leqslant f(y),$$

which implies the claim. □

Proof of Theorem 4.4.10 (Mazur–Bourgin theorem). Let N be a closed convex subset of the LCTVS E. Let x be a weak cluster point of N. We have to show that $x \in N$. We prove it by contradiction.

Suppose that $x \notin N$. By Proposition 4.4.16, there exists a continuous functional g and a $\delta > 0$ so that $\operatorname{Re}\bigl(g(x)\bigr) + \delta \leqslant \operatorname{Re}\bigl(g(y)\bigr)$ holds for all $y \in N$. But then, one has

$$|g(y) - g(x)| \geqslant \delta \quad \text{for all } y \in N,$$

and x is not a weak cluster point of N, which is a contradiction. □

4.4.3. The Eberlein–Šmulian theorem

In dealing with weak almost periodicity, we are dealing with compactness in the weak topology of Banach spaces. In this section, we derive a theorem of Eberlein–Šmulian, which allows us to work with sequences when proving weak almost periodicity. The proof presented here follows Whitley's exposition [51]; see also [36].

A subset A in a topological space E is said to have the *convergent subsequence property* if every sequence $\{a_n\}_n$ with $a_n \in A$ has a subsequence $\{a_{k_n}\}$ convergent to some $a \in E$. If, in addition, there always exists such a subsequence for which $a \in A$, then A is said to be *sequentially compact*. It is well known that compactness and sequential compactness are equivalent in metric spaces, while they are not related in general. It is easy to check that the convergent subsequence property is equivalent to having sequentially compact closure in metric spaces, but in general the former is weaker.

The weak topology of a Banach space $(E, \|.\|)$ is usually not metrisable, and hence we should not expect any relation between compactness and sequential compactness. Yet, the Eberlein–Šmulian theorem below shows that the two concepts are equivalent in this case. The reason why this happens is that, while the weak topology is not metrisable, we can prove that, if $A \subset E$ is a weakly compact set and E is separable, the restriction of the weak topology to A becomes metrisable.

Lemma 4.4.17. *Let $E \neq \{0\}$ be a Banach space, and let $A \subset E$.*

(i) *If A is weakly compact, then A is bounded.*

(ii) *If A has the convergent subsequence property in the weak topology, then A is weakly bounded and bounded. In particular, if A is weakly sequentially compact, then A is bounded.*

Proof. Claim (i) is almost immediate: As any functional is weakly continuous, the compactness of A implies that every functional is bounded on A, i.e., A is weakly bounded. Lemma 4.4.9 completes the claim.

To establish claim (ii), it is again sufficient to prove that A is weakly bounded. Assume in contradiction that A is not weakly bounded. Then, there exists some $\phi \in E'$ which is not bounded on A. Now, for each n, there exists some $a_n \in A$ such that

$$|\phi(a_n)| > n.$$

As $\{a_n\} \subset A$ and A has the convergent subsequence property, there exists a subsequence $\{a_{k_n}\}$ and some $a \in E$ such that

$$\{a_{k_n}\} \xrightarrow{\text{weakly}} a,$$

which gives

$$\{\phi(a_{k_n})\} \longrightarrow \phi(a) \quad \text{in } \mathbb{C},$$

contrary to $\{|\phi(a_{k_n})|\} \to \infty$. Therefore, A is weakly bounded, and hence bounded. □

Lemma 4.4.18. *Let E be a separable Banach space, and let $M \subset E$ be weakly compact. Then, the weak topology on M is metrisable.*

PROOF. Let $\{x_n\}$ be a sequence of non-zero elements of E which is dense in E. For each n, by Theorem 4.4.3 (Hahn–Banach), we can pick some $\phi_n \in E'$ such that

$$|\phi_n(x_n)| = \|x_n\| \quad \text{and} \quad \|\phi_n\| = 1.$$

Now, let us define $d\colon E\times E \longrightarrow \mathbb{R}$ by

$$d(x,y) := \sum_{n=1}^{\infty} \frac{1}{2^n} |\phi_n(x-y)|.$$

The function d is well defined,

$$d(x,y) \leqslant \sum_{n=1}^{\infty} \frac{1}{2^n} \|\phi_n\| \|x-y\| = \|x-y\| < \infty,$$

since $\|\phi_n\| = 1$.

Let us next prove that d is a metric on E in three steps.

First, $d(x,y) \geqslant 0$ follows immediately from the definition. Moreover, if $d(x,y) = 0$ for some $x, y \in E$, we have $\phi_n(x-y) = 0$ for all n. Let $\varepsilon > 0$. Then, by the denseness of the sequence $\{x_n\}$, there exists some n such that

$$\|(x-y) - x_n\| < \varepsilon.$$

Since $\phi_n(x-y) = 0$, we get

$$\begin{aligned} \|x_n\| &= |\phi_n(x_n)| = |\phi_n(x_n) - \phi_n(x-y)| = |\phi_n(x_n - (x-y))| \\ &\leqslant \|\phi_n\| \, \|(x-y) - x_n\| < \varepsilon, \end{aligned}$$

from which

$$\|x-y\| \leqslant \|(x-y) - x_n\| + \|x_n\| < 2\varepsilon.$$

This shows that $\|x-y\| < 2\varepsilon$ for all $\varepsilon > 0$, and hence $\|x-y\| = 0$, which means $x = y$.

Second, the symmetry relation $d(x,y) = d(y,x)$ is straightforward, as $|\phi_n(x-y)| = |\phi_n(y-x)|$ holds for all n.

Third, the triangle inequality $d(x,y) \leqslant d(x,z) + d(z,y)$ is also simple. Indeed, if $x, y, z \in M$, one gets

$$\begin{aligned} d(x,y) &= \sum_{n=1}^{\infty} \frac{1}{2^n} |\phi_n(x-y)| = \sum_{n=1}^{\infty} \frac{1}{2^n} |\phi_n(x-z) + \phi_n(z-y)| \\ &\leqslant \sum_{n=1}^{\infty} \frac{1}{2^n} \big(|\phi_n(x-z)| + |\phi_n(z-y)| \big) \\ &= \sum_{n=1}^{\infty} \frac{1}{2^n} |\phi_n(x-z)| + \sum_{n=1}^{\infty} \frac{1}{2^n} |\phi_n(z-y)| \\ &= d(x,z) + d(z,y). \end{aligned}$$

This completes the argument that d is a metric on E.

Next, we claim the continuity of the identity map

$$\mathrm{id}\colon (M, \text{weak}) \longrightarrow (M, d).$$

First, since M is weakly compact, it is bounded by Lemma 4.4.17(i). Therefore, there exists some C such that $\|a\| \leqslant C$ for all $a \in M$. Now, let $U \subset M$ be open in the metric topology. Then, for each $a \in U$, there exists some $\varepsilon > 0$ such that $B_\varepsilon(a) \subseteq U$. Fix some $N \in \mathbb{N}$ such that $\frac{C}{2^{N-1}} < \frac{\varepsilon}{2}$, and define

$$V := \big\{x \in M : \big|\phi_j(x-a)\big| \leqslant \frac{\varepsilon}{2} \text{ for all } 1 \leqslant j \leqslant N\big\}.$$

Then, V is a weakly open set. We next show that $V \subseteq B_\varepsilon(a) \subseteq U$. This will establish that U is weakly open, and hence that the map id is continuous.

Let $x \in V$. Then, since $x, a \in M$,

$$\begin{aligned}
d(x,a) &= \sum_{n=1}^{\infty} \frac{1}{2^n} |\phi_n(x-a)| \\
&= \sum_{n \leqslant N} \frac{1}{2^n} |\phi_n(x-a)| + \sum_{n>N} \frac{1}{2^n} |\phi_n(x-a)| \\
&\leqslant \sum_{n \leqslant N} \frac{1}{2^n} \frac{\varepsilon}{2} + \sum_{n>N} \frac{1}{2^n} \|\phi_n\| \|x-a\| \\
&\leqslant \frac{\varepsilon}{2} + \sum_{n>N} \frac{1}{2^n} \big(\|x\| + \|a\|\big) \leqslant \frac{\varepsilon}{2} + \sum_{n>N} \frac{2C}{2^n} \\
&= \frac{\varepsilon}{2} + \frac{2C}{2^N} < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon,
\end{aligned}$$

which implies the continuity of id.

Now, it is easy to see that id is a homeomorphism. Since (M, d) is a Hausdorff space, its compact subsets are closed. Since M is weakly compact and id is weakly continuous, id maps weakly closed subsets of M onto compact, hence closed, subsets of (M, d). This shows that id is a closed map, and since id is a bijection, it is a homeomorphism.

This shows that the weak topology on M is induced by d, and therefore metrisable. □

We can now relate weak compactness with weak sequential compactness as follows.

Theorem 4.4.19 (Šmulian)**.** *Let E be a Banach space and let $M \subset E$ be a weakly compact subset. Then, M is weakly sequentially compact.*

PROOF. Let $\{x_n\} \subset M$ be a sequence and let

$$F := \overline{\operatorname{span}\{x_n\}}^{\|\cdot\|},$$

where the closure is with respect to the norm. Since F is a closed subspace, it is weakly closed by Corollary 4.4.11. Then, $M \cap F$ is weakly closed in M and hence weakly compact.

Thus, $M \cap F$ is a weakly compact set in the *separable* Banach space F, and hence, by Lemma 4.4.18, $M \cap F$ is weakly sequentially compact. Therefore, the sequence $\{x_n\}$ has a subsequence convergent to some $x \in M \cap F$, which establishes the claim. □

To complete this section, we prove that the converse of Šmulian's theorem is also true. To do so, we first need a preparatory lemma.

Lemma 4.4.20. *Let $(E, \|.\|)$ be a Banach space and let $J\colon E \hookrightarrow E''$ be the canonical embedding into its bi-dual from Eq.* (4.4.3)*. Then, a set $M \subset E$ is weakly compact if and only if M is bounded and $J(M) \subset E''$ is weak-$*$ closed.*

PROOF. By the definition of the weak topology on E, and of the weak-$*$ topology on E'', for $\{x_\alpha\} \subset E$ and $x \in E$ we have $\{x_\alpha\} \xrightarrow{\text{weakly}} x$ if and only if $\{J(x_\alpha)\} \xrightarrow{\text{weak-}*} J(x)$.

$\Longrightarrow$: Since M is weakly compact, it is bounded by Lemma 4.4.17. Suppose that $\{J(x_\alpha)\} \xrightarrow{\text{weak-}*} y$ in E''. Since $\{x_\alpha\} \subset M$ and M is weakly compact, $\{x_\alpha\}$ has a subnet $\{x_\beta\}$ which converges to some $x \in M$, from which we conclude that $\{J(x_\beta)\} \longrightarrow J(x)$ and $y = J(x) \in J(M)$.

$\Longleftarrow$: Let $\{x_\alpha\}$ be a net in M. Since M is bounded, $J(M)$ has weak-$*$ compact closure by Theorem 4.4.6 (Banach–Alaoglu). Since $J(M)$ is assumed to be weak-$*$ closed, it is weak-$*$ compact. Therefore, the net $\{J(x_\alpha)\}$ has a subnet $\{J(x_\beta)\}$ which is weak-$*$ convergent to some $y \in J(M)$. Then, $y = J(x)$ for some $x \in M$, and $\{x_\beta\}$ converges weakly to the point $x \in M$. □

We can now prove the converse of Šmulian's theorem.

Theorem 4.4.21 (Eberlein)**.** *Let E be a Banach space and let $A \subset E$ have the convergent subsequence property in the weak topology. Then, the weak closure of A in E is weakly compact. In particular, if A is weakly sequentially compact, then it is weakly compact.*

PROOF. By Lemma 4.4.17, A is weakly bounded. Let M be the weak closure of A. It too is weakly bounded, and hence also bounded by Lemma 4.4.9. Therefore, by Lemma 4.4.20, it suffices to show that the image $J(M)$ of M under the canonical embedding $J\colon E \hookrightarrow E''$ is weak-$*$ closed in E''. Denote

by B the weak-$*$ closure of $J(M)$ in E'' and let $y \in B$. We need to show that $y \in J(M)$.

To do so, we construct inductively a sequence of elements $x_n \in A$ and finite sets $F_n \subset E'$ such that,

(i) for all n and for all $\phi \in F_n$, we have $\|\phi\| = 1$;

(ii) for all n and all $\phi \in F_1 \cup F_2 \cup \cdots \cup F_n$, we have

$$|(y - J(x_n))(\phi)| < \frac{1}{n};$$

(iii) for all $z \in \operatorname{span}\{y, J(x_1), J(x_2), \ldots, J(x_{n-1})\}$, we have

$$\frac{\|z\|}{2} \leqslant \max\big\{|z(\phi)| : \phi \in F_n\big\}.$$

We start by picking some $\phi_1 \in E'$ with $\|\phi_1\| = 1$ such that

$$|y(\phi_1)| \geqslant \frac{\|y\|}{2}.$$

Next, using the weak-$*$ denseness of $J(M)$ in B, we choose $u_1 \in M$ such that

$$|(y - J(u_1))(\phi_1)| < \frac{1}{2}.$$

Since A is weakly dense in M, there exists $x_1 \in A$ with $|\phi_1(x_1) - \phi_1(u_1)| < \frac{1}{2}$. This can be rewritten as $|J(x_1)(\phi_1) - J(u_1)(\phi_1)| < \frac{1}{2}$, and we obtain

$$|(y - J(x_1))(\phi_1)| < 1.$$

Clearly, (i), (ii) and (iii) hold at level $n = 1$.

Supposing that $x_1, \ldots, x_{n-1}$ and $F_1, \ldots, F_{n-1}$ are available, we construct x_n and F_n as follows. First, let us note that

$$V := \operatorname{span}\big\{y, J(x_1), J(x_2), \ldots, J(x_{n-1})\big\}$$

is a finite-dimensional subspace of E''. Therefore, the unit sphere

$$\mathbb{S} := \{z \in V : \|z\| = 1\}$$

is compact in V. Covering this sphere by open balls of radius $\frac{1}{4}$, we can find some $z_1, \ldots, z_m \in \mathbb{S}$ such that every $z \in \mathbb{S}$ is within distance $\frac{1}{4}$ of some z_k.

Now, for each $1 \leqslant k \leqslant m$ choose some $\phi_k \in E'$ with $\|\phi_k\| = 1$ such that

$$|z_k(\phi_k)| > \frac{3}{4}.$$

We set $F_n := \{\phi_1, \ldots, \phi_m\}$. Since the set $F_1 \cup F_2 \cup \cdots \cup F_n$ is finite, $J(M)$ is weak-$*$ dense in B and A is weakly dense in M, we can find some $x_n \in A$ such that

$$|(y - J(x_n))(\phi)| < \frac{1}{n},$$

for all $\phi \in F_1 \cup F_2 \cup \cdots \cup F_n$.

By construction, $x_1, \ldots, x_n$ and $F_1, \ldots, F_n$ satisfy conditions (i) and (ii). To check (iii), let $z \in \operatorname{span}\{y, J(x_1), J(x_2), \ldots, J(x_{n-1})\} = V$. If $z = 0$, the

condition (iii) is trivially satisfied. For $z \neq 0$, we can assume that $\|z\| = 1$, so $z \in \mathbb{S}$. There exists some $1 \leqslant k \leqslant m$ so that

$$\|z - z_k\| < \frac{1}{4}.$$

Then,

$$|(z - z_k)(\phi_k)| < \|z - z_k\|\|\phi_k\| < \frac{1}{4},$$

and hence

$$|z(\phi_k)| \geqslant |(z_k)(\phi_k)| - |(z - z_k)(\phi_k)| > \frac{3}{4} - \frac{1}{4} = \frac{1}{2}.$$

This implies the estimate

$$|z(\phi_k)| \geqslant \frac{\|z\|}{2},$$

which proves (iii) and finishes the construction of the sequence $\{x_n\}$.

By the weak convergent subsequence property of A, the sequence $\{x_n\}$ has a subsequence $\{x_{k_n}\}$ that converges weakly to some $x \in M$. We claim that $J(x) = y$, which will then complete the proof of the theorem.

Let $\varepsilon > 0$, and let $\phi \in \bigcup_{n=1}^{\infty} F_n$. Then, $\phi \in F_{n_0}$ for some n_0. Pick $N > n_0$ so that $\frac{1}{N} < \frac{\varepsilon}{2}$. Since $\{x_{k_n}\} \longrightarrow x$ weakly, there exists some $N_1 > N$ so that, if $k_n > N_1$, we have $\big|\phi(x_{k_n} - x)\big| < \frac{\varepsilon}{2}$. With such a k_n, property (ii) gives

$$\begin{aligned} |(y - J(x))\,(\phi)| &\leqslant \big|\big(y - J(x_{k_n})\big)\,(\phi)\big| + \big|\big(J(x_{k_n}) - J(x)\big)\,(\phi)\big| \\ &\leqslant \frac{1}{k_n} + |\phi(x_n - x)| < \varepsilon. \end{aligned}$$

This shows that, for all $\varepsilon > 0$, we have

$$|(y - J(x))(\phi)| < \varepsilon,$$

and hence $|(y - J(x))(\phi)| = 0$, which is true for all $\phi \in \bigcup_{n=1}^{\infty} F_n$.

We claim that this implies $y - J(x) = 0$. Indeed, by (iii), we have

$$\|z\| \leqslant 2 \max\big\{|z(\phi)| : \phi \in F_n\big\}$$

for all $z \in \operatorname{span}\{y, J(x_1), J(x_2), \ldots, J(x_{n-1})\}$, and therefore

$$\|z\| \leqslant 2 \sup\left\{|z(\phi)| : \phi \in \bigcup_{n=1}^{\infty} F_n\right\}. \tag{4.4.6}$$

Since the right-hand side of Eq. (4.4.6) does not depend on n, it holds for all $z \in \operatorname{span}\big(\{y\} \cup \{J(x_n)\}_n\big)$, and hence also for all z in the norm closure, which means

$$z \in \overline{\operatorname{span}\big(\{y\} \cup \{J(x_n)\}_n\big)}^{\|\cdot\|}.$$

Since this subspace is closed, hence weakly closed (Corollary 4.4.11), and since x is in the weak closure of $\{x_n\}$, it follows that it contains $y - J(x)$. Therefore, setting $z = y - J(x)$ in Eq. (4.4.6), we get

$$\|y - J(x)\| \leqslant 2 \sup\left\{ |(y - J(x))(\phi)| : \phi \in \bigcup_{n=1}^{\infty} F_n \right\} = 0,$$

so $J(x) = y$ as claimed. □

By combining Eberlein's theorem with that of Šmulian, we get the following statement.

Theorem 4.4.22 (Eberlein–Šmulian)**.** *Let E be a Banach space and let the set $M \subset E$ be weakly closed. Then, M is weakly compact if and only if M is weakly sequentially compact.* □

In fact, Theorem 4.4.21 is slightly stronger than the 'only if' part of this theorem, and we can deduce from it the following useful criterion for weak almost periodicity.

Proposition 4.4.23. *Let $f \in C_{\mathsf{u}}(G)$. Then $f \in \mathrm{WAP}(G)$ if and only if, for each sequence $\{t_n\}$ with $t_n \in G$, there exists a subsequence $\{t_{k_n}\}$ and some $g \in C_{\mathsf{u}}(G)$ such that $\{t_{k_n}.f\} \xrightarrow{\text{weakly}} g$.*

Proof. We have $f \in \mathrm{WAP}(G)$ if and only if $\overline{G.f}$ is weakly compact in $C_{\mathsf{u}}(G)$. By Theorem 4.4.21, this is equivalent to the convergent subsequence property of $G.f$. □

For completeness, we add the corresponding criteria for strong almost periodicity.

Proposition 4.4.24. *Let $f \in C_{\mathsf{u}}(G)$. Then, $f \in \mathrm{SAP}(G)$ if and only if, for each sequence $\{t_n\}$ with $t_n \in G$, there exists a subsequence $\{t_{k_n}\}$ such that $\{t_{k_n}.f\}$ is Cauchy in $(C_{\mathsf{u}}(G), \|.\|_\infty)$.*

Proof. Since $(C_{\mathsf{u}}(G), \|.\|_\infty)$ is a Banach space, thus metrisable, the norm closure $\overline{G.f}$ is compact if and only if $\overline{G.f}$ is sequentially compact.

$\Longrightarrow$: Since $\{t_n.f\} \subset \overline{G.f}$ and $\overline{G.f}$ is sequentially compact, $\{t_n.f\}$ has a subsequence $\{t_{k_n}.f\}$ that is convergent in $\overline{G.f}$. In particular, $\{t_{k_n}.f\}$ is Cauchy.

$\Longleftarrow$: We need to prove that $\overline{G.f}$ is sequentially compact in $(C_{\mathsf{u}}(G), \|.\|_\infty)$. Let $\{g_n\} \in \overline{G.f}$ be any sequence. Then, by the definition of $\overline{G.f}$, for each n we can find some $t_n \in G$ such that

$$\|t_n.f - g_n\|_\infty \leqslant \frac{1}{n}.$$

By the hypothesis, $\{t_n\}$ has a subsequence $\{t_{k_n}\}$ such that $\{t_{k_n}.f\}$ is Cauchy in $(C_{\mathsf{u}}(G), \|.\|_\infty)$, and since $(C_{\mathsf{u}}(G), \|.\|_\infty)$ is a Banach space, there is a function $g \in C_{\mathsf{u}}(G)$ such that

$$t_{k_n}.f \longrightarrow g.$$

Then, $g_{k_n} \longrightarrow g \in \overline{G.f}$, which is what we wished to prove. □

4.4.4. Convex hulls

In this section, we derive an important characterisation of almost periodicity in terms of convex hulls of orbits.

Lemma 4.4.25. *Let E be an LCTVS and let $x_1, \ldots, x_n \in E$. Then, the convex hull of $\{x_1, \ldots, x_n\}$ is compact.*

Proof. Let $f\colon \mathbb{R}^n \longrightarrow E$ be the continuous mapping defined by

$$f(a_1, \ldots, a_n) := a_1x_1 + \cdots + a_nx_n.$$

Since the set $S := \big\{(a_1, \ldots, a_n) \in [0,1]^n : a_1 + \cdots + a_n = 1\big\}$ is compact, $f(S)$, which is the convex hull of $\{x_1, \ldots, x_n\}$, is also compact. □

Theorem 4.4.26 (Krein–Šmulian [13, 52])**.** *Let E be a Banach space and let $M \subset E$ be weakly compact. Then, the closed convex hull of M is weakly compact.*

Our proof is based on [52]. But before starting the proof, it is useful to make some preliminary observations. The first of these is that it suffices to prove the theorem in the case when E is separable. To see this, let

$$\mathcal{C}(M) := \left\{\sum_{k=1}^{n} a_kt_k : n \geqslant 1,\, t_k \in M,\, a_k \in [0,1],\, \sum_{k=1}^{n} a_k = 1\right\}$$

be the convex hull of M and let $\overline{\mathcal{C}(M)}$ be its norm closure. By Theorem 4.4.10 (Mazur–Bourgin), $\overline{\mathcal{C}(M)}$ is also the weak closure of $\mathcal{C}(M)$. We want to prove that $\overline{\mathcal{C}(M)}$ is weakly compact. By Theorem 4.4.22 (Eberlein–Šmulian), it suffices to prove that $\overline{\mathcal{C}(M)}$ is weakly sequentially compact.

With that in mind, let $\{x_n\} \subset \overline{\mathcal{C}(M)}$. Then, since $\overline{\mathcal{C}(M)}$ is the norm closure of $\mathcal{C}(M)$, there exists some $y_n \in \mathcal{C}(M)$ such that

$$\|x_n - y_n\| \leqslant \frac{1}{n}.$$

Since $\{x_n - y_n\}$ converges to 0 in norm, it also converges weakly to 0. If we can prove that y_n has a subsequence y_{k_n} that converges weakly to some $y \in \overline{\mathcal{C}(M)}$, it follows that

$$x_{k_n} \xrightarrow{\text{weakly}} y,$$

which is what we need. So, what we really have to show is that every sequence $\{y_n\}$ in $\mathcal{C}(M)$ has a subsequence that is weakly convergent to some $y \in \overline{\mathcal{C}(M)}$.

Suppose then that $\{y_n\}$ is a sequence in $\mathcal{C}(M)$. Since $y_n \in \mathcal{C}(M)$ for any $n \in \mathbb{N}$, we can write

$$y_n = \sum_{j=1}^{m_n} a_{n,j} z_{n,j}$$

for some $z_{n,j} \in M$ and $a_{n,j} \in [0,1]$ with $\sum_{j=1}^{m_n} a_{n,j} = 1$.

Next, consider the norm closure

$$F := \overline{\operatorname{span}\{z_{n,j} : n \geqslant 1,\, 1 \leqslant j \leqslant m_n\}}.$$

Then, F is closed subspace of E and therefore weakly closed. Thus, the set

$$M_0 := F \cap M$$

is weakly closed in M and therefore weakly compact. Since all of the elements $y_n \in \mathcal{C}(M_0) \subset F$, the desired point y will be in $\overline{\mathcal{C}(M_0)}$. Moreover, F is a separable Banach space. Thus, our problem reduces to a problem in separable spaces, and so we can restrict to that case and assume from the outset that E is separable.

The second observation involves the canonical embedding

$$J\colon E \hookrightarrow E''$$

of a Banach space into its bi-dual. The question involves identifying elements of $J(E)$. Ultimately, the proof of the Krein–Šmulian theorem depends on the weak compactness of the unit ball in $C(M)'$, where $C(M)$ denotes the space of continuous functions on M, and transferring this information back to E. The mapping J plays an essential role in this.

Lemma 4.4.27. *Let E be a separable Banach space and let $x'' \in E''$ (the bi-dual of E). Suppose that, for each sequence $\{x'_n\} \subset E'$ that weak-$*$ converges to some $x' \in E'$, we have $\{x''(x'_n)\} \longrightarrow x''(x')$. Then, $x'' \in J(E)$.*

Proof.[6] Since E is separable, it has a countable dense subset $\{x_k\}$. Now, J is an isometric embedding of E into E'', so $J(E)$ is a closed subset of E''. Suppose, by way of contradiction, that $x'' \notin J(E)$. As a consequence, we have $d := \inf\{\|x'' - J(x)\| : x \in E\} > 0$. By Theorem 4.4.3 (Hahn–Banach), there is x''' of norm 1 in E''' with $x'''(J(E)) = 0$ and $x'''(x'') = d$.

Take any $n \in \mathbb{N}$ and compare the two ordered sets

$$\begin{aligned} &\{x'''(x''), x'''(J(x_1)), \ \dots\ , x'''(J(x_n))\} \\ &\{\ x''(x'), \quad x'(x_1), \quad \dots\ , \quad x'(x_n)\quad \} \end{aligned}$$

where $x'''(x'') = d$ and $x'''(J(x_i)) = 0$ for all $1 \leqslant i \leqslant n$. Using Theorem 4.4.5 (Goldstine), we can choose elements $x' \in B'$ (the unit ball in E') to make

[6] Since this proof involves E, E', E'', E''', we follow not only the proof, but also the notation of [52], which makes it easy to see where all the elements lie.

these two sets of values as close as we please. In particular, we can find $x'_n \in E'$ so that

$$\|x'_n\| \leqslant 1, \quad x''(x'_n) \geqslant \frac{d}{2}, \quad \text{and} \quad |x'_n(x_i)| < 1 \text{ for all } 1 \leqslant i \leqslant n.$$

This way, we have constructed a sequence $\{x'_n\} \subset E'$. Not surprisingly, one has $\{x'_n\} \xrightarrow{\text{weak-}*} 0$. Indeed, choose any $z \in E$ and any $\varepsilon > 0$. By the denseness of the sequence $\{x_i\}$, we can find x_j with $\|z/\varepsilon - x_j\| < 1$. Then, for all $n \geqslant j$,

$$\begin{aligned} |x'_n(z)| &= \varepsilon \left|x'_n\left(\tfrac{z}{\varepsilon}\right)\right| = \varepsilon \left|x'_n\left(\tfrac{z}{\varepsilon}\right) - x'_n(x_j) + x'_n(x_j)\right| \\ &\leqslant \varepsilon \|x'_n\| \left\|\tfrac{z}{\varepsilon} - x_j\right\| + \varepsilon \left|x'_n(x_j)\right| \leqslant 2\varepsilon. \end{aligned}$$

This shows that $\{x'_n\} \xrightarrow{\text{weak-}*} 0$.

By the hypothesis of our lemma, we would now have the convergence $\{x''(x'_n)\} \longrightarrow x''(0) = 0$, which is impossible since $x''(x'_n) \geqslant d/2$ for all n. This proves that $x'' \in J(E)$. □

Proof of Theorem 4.4.26 (Krein–Šmulian theorem). In view of our above remarks, we are assuming that E is separable and that $M \subset E$ is a weakly compact subset. Consider the Banach space $(C(M), \|.\|_\infty)$ of continuous functions on M, where the continuity is with respect to the *weak* topology of M. By the Riesz–Markov theorem [42, Thm. 6.19] (see also Theorem 4.9.3 below), the dual space $C(M)'$ of this space is the space of regular Borel measures on the compact set M. Furthermore, the weak-$*$ topology of $C(M)'$ is precisely the vague topology when $C(M)'$ is interpreted as a space of measures. In particular, the unit ball (in the norm topology of $C(M)'$) is weak-$*$ compact by Theorem 4.4.6 (Banach–Alaoglu). It is this compactness that we are now going to exploit by creating a mapping from $C(M)'$ back to E.

Let $R: E' \longrightarrow C(M)$ be defined by restriction, $(R\phi)(x) = \phi(x)$, for $\phi \in E'$ and $x \in M$. This mapping is weak-$*$ continuous. Given R, we also have its conjugate mapping

$$R^*: C(M)' \longrightarrow E'',$$

which is continuous with respect to the weak-$*$ topologies.

We now are going to use Lemma 4.4.27 to show the crucial fact that $R^*(C(M)') \subseteq J(E)$ (recall that $J: E \hookrightarrow E''$ is the natural embedding). Note that, for all $u \in M$, $J(u)$ is the evaluation of functions at u, i.e., the Dirac measure δ_u.

For this purpose, let $\{x'_n\} \subset E'$ be any sequence that is weak-$*$ convergent to some element $x \in E'$. Consider any $\mu \in C(M)'$, which we will think of as a regular measure. By Lemma 4.4.9, the set $\{x'_n\}$ is bounded. Thus, by the

dominated convergence theorem of measure theory, we have

$$(R^*\mu)(x'_n) \,=\, \int_M x'_n(k)\,\mathrm{d}\mu(k) \;\xrightarrow{n\to\infty}\; \int_M x(k)\,\mathrm{d}\mu(k) \,=\, (R^*\mu)(x').$$

Therefore, by Lemma 4.4.27, we obtain that $\mu \in J(E)$.

Since $J\colon E \hookrightarrow J(E)$ is a bijection, it has an inverse, $J^{-1}\colon J(E) \longrightarrow E$. It follows from its definition that J^{-1} is weak-$*$ to weak continuous. We therefore get a mapping $J^{-1} \circ R^*\colon C(M)' \longrightarrow E$, which is weak-$*$ to weak continuous.

Next, let us observe that, for all $a \in M$, the regular Borel measure $\delta_a \in C(M)'$ and, since $|\delta_a(\phi)| = |\phi(a)| \leqslant \|\phi\|_\infty$ for all $\phi \in C(M)$, we have $\|\delta_a\|_\infty \leqslant 1$. (In fact, using Theorem 4.4.3 (Hahn–Banach), we can see that $\|\delta_a\|_\infty = 1$.) Therefore, δ_a lies in the closed unit ball of $C(M)'$ and $\big(J^{-1} \circ R^*\big)(\delta_a) = a$.

The unit ball in $C(M)'$ is a convex and weak-$*$ compact set, and it is mapped by $J^{-1} \circ R^*$ onto a convex and weakly compact subset of E. This subset contains M itself, and so also the closed convex hull of M, which is thus weakly compact. This proves the theorem. □

Specialising to $C_{\mathsf{u}}(G)$ with its strong and weak topologies, respectively, and recalling the definition of $\mathcal{C}_f$ in Eq. (4.4.5), we obtain the following consequence.

Theorem 4.4.28. *Let $f \in C_{\mathsf{u}}(G)$. Then,*

(i) *f is weakly almost periodic if and only if $\mathcal{C}_f$ is weakly compact in $C_{\mathsf{u}}(G)$;*

(ii) *f is strongly almost periodic if and only if $\mathcal{C}_f$ is compact in $(C_{\mathsf{u}}(G), \|.\|_\infty)$.*

Proof. We first show claim (i).

$\Longleftarrow$: Recall that $\mathcal{C}_f$ denotes the closed convex hull of f and that $\mathcal{R}^* = \mathcal{G}^*$ in this case. Since $G.f \subseteq \mathcal{C}_f$ and since $\mathcal{C}_f$ is weakly compact, it follows that the weak closure $\overline{G.f}^{\mathsf{w}} \subseteq \mathcal{C}_f$ is weakly compact.

$\Longrightarrow$: This follows from Theorem 4.4.26 (Krein–Šmulian).

Let us turn to claim (ii).

$\Longleftarrow$: Since $G.f \subseteq \mathcal{C}_f$ and since $\mathcal{C}_f$ is compact, it follows that the norm closure $\overline{G.f} \subseteq \mathcal{C}_f$ is compact.

$\Longrightarrow$: Since $(C_{\mathsf{u}}(G), \|.\|_\infty)$ is complete, it suffices to show the total boundedness of the convex hull $\mathcal{C}\big(\overline{G.f}\big)$ of $\overline{G.f}$ in order to prove compactness of $\mathcal{C}_f$. That is, we show that, for any $\varepsilon > 0$, we can find $g_1, \ldots, g_m \in O_f$ so that

$$\mathcal{C}\big(\overline{G.f}\big) \,\subseteq\, \bigcup_{j=1}^{m} B_\varepsilon(g_j). \tag{4.4.7}$$

Since $\overline{G.f}$ is compact, there are $h_1, \dots, h_\ell \in \overline{G.f}$ so that

$$\overline{G.f} \subseteq \bigcup_{j=1}^{\ell} B_{\frac{\varepsilon}{2}}(h_j).$$

By Lemma 4.4.25, the convex hull $\mathcal{C}(h_1, \dots, h_\ell)$ of $\{h_1, \dots, h_\ell\}$ is compact. Thus, there exist $g_1, \dots, g_m \in \mathcal{C}(h_1, \dots, h_\ell)$ so that

$$\mathcal{C}(h_1, \dots, h_\ell) \subseteq \bigcup_{j=1}^{m} B_{\frac{\varepsilon}{2}}(g_j). \tag{4.4.8}$$

We now show that Eq. (4.4.7) holds for these functions $g_1, \dots, g_m$. To this end, let $h \in \mathcal{C}\big(\overline{G.f}\big)$. Since $\mathcal{C}\big(\overline{G.f}\big)$ is the convex hull of $\overline{G.f}$, we now have $h = \sum_{i=1}^{s} a_i h_i'$ for some $h_i' \in \overline{G.f}$ and some $a_1, \dots, a_s \in [0,1]$ with $a_1 + \cdots + a_s = 1$. Note that each $h_i' \in B_{\frac{\varepsilon}{2}}(g_{n_i})$ for some $g_{n_i} \in \{g_1, \dots, g_m\}$. Consequently, $g' := a_1 g_{n_1} + \cdots + a_s g_{n_s} \in \mathcal{C}(g_1, \dots, g_m) \subseteq \mathcal{C}(h_1, \dots, h_\ell)$, so $g' \in B_{\frac{\varepsilon}{2}}(g_k)$ for some g_k from Eq. (4.4.8).

Finally, putting the pieces together, we get

$$\|h - g_k\|_\infty \leqslant \|h - g'\|_\infty + \|g' - g_k\|_\infty \leqslant \sum_{i=1}^{s} a_i \|h_i' - g_{n_i}\|_\infty + \frac{\varepsilon}{2} < \varepsilon.$$

Thus, $h \in B_\varepsilon(g_k)$, which proves Eq. (4.4.7). □

4.4.5. Stone–Čech compactification

In this section, we provide proofs for the last two statements of Proposition 4.3.11. The key device is the Stone–Čech compactification $\mathrm{SC}(G)$ of an LCAG G, by which we see that weak convergence in $C_{\mathsf{u}}(G)$ is equivalent to equi-boundedness and pointwise convergence in $C(\mathrm{SC}(G))$. Details about this type of compactification can be found in [23]. In outline, we take one copy $[0,1]_F$ of the unit interval for each continuous function $F\colon G \longrightarrow [0,1]$. Then, taking the product of all such $[0,1]_F$,

$$P := \prod_F [0,1]_F,$$

with the usual product topology, we obtain a compact space. Furthermore, G embeds into it with $x \in G$ going to the element $j(x)$ in P whose F-component is $F(x)$, which means we have a mapping $j\colon G \hookrightarrow \mathrm{SC}(G)$. The closure of the image of G in P is the Stone–Čech compactification $\mathrm{SC}(G)$ of G. The action T of G on itself extends to a continuous action of G on $\mathrm{SC}(G)$. The main feature of $\mathrm{SC}(G)$ is that every bounded and continuous $\mathbb{C}$-valued function f on G extends uniquely to a continuous $\mathbb{C}$-valued function f_{SC} on $\mathrm{SC}(G)$,

and the sup-norms of each are the same.[7] This establishes a normed space G-equivariant isomorphism

$$C_{\mathsf{b}}(G) \simeq C\big(\mathrm{SC}(G)\big), \tag{4.4.9}$$

where $C_{\mathsf{b}}(G)$ denotes the space of all bounded continuous functions from G to $\mathbb{C}$ as usual.

The inclusion $C_{\mathsf{u}}(G) \subseteq C_{\mathsf{b}}(G)$ then induces a norm-preserving embedding

$$i_{\mathrm{SC}}\colon (C_{\mathsf{u}}(G), \|.\|) \hookrightarrow (C\big(\mathrm{SC}(G)\big), \|.\|),$$

the norm $\|.\|$ in each case being the sup-norm $\|.\|_\infty$. Therefore, we get the following result.

Theorem 4.4.29. *The embedding $j\colon G \hookrightarrow \mathrm{SC}(G)$ induces a norm-preserving embedding*

$$i_{\mathrm{SC}}\colon (C_{\mathsf{u}}(G), \|.\|) \hookrightarrow (C\big(\mathrm{SC}(G)\big), \|.\|)$$

such that $\big(i_{\mathrm{SC}}(f)\big)\big(j(x)\big) = f(x)$ for all $f, g \in C_{\mathsf{u}}(G)$ and $x \in G$. Furthermore,

(i) *$i_{\mathrm{SC}}(fg) = i_{\mathrm{SC}}(f)\, i_{\mathrm{SC}}(g)$ for all $f, g \in C_{\mathsf{u}}(G)$, and*
(ii) *for any sequence $\{f_n\} \subset C_{\mathsf{u}}(G)$ and any $f \in C_{\mathsf{u}}(G)$,*

$$\{f_n\} \xrightarrow{\textit{weakly}} f \quad\Longleftrightarrow\quad \{i_{\mathrm{SC}}(f_n)\} \xrightarrow[C(\mathrm{SC}(G))]{\textit{weakly in}} i_{\mathrm{SC}}(f).$$

Proof. The existence of i_{SC} is evident from the above construction, and property (i) is clear from the definitions.

As for (ii), i_{SC} is a norm-preserving isomorphism between $(C_{\mathsf{u}}(G), \|.\|)$ and $(i_{\mathrm{SC}}(C_{\mathsf{u}}(G)), \|.\|)$. Since $(C_{\mathsf{u}}(G), \|.\|)$ is a Banach space, it follows that $(i_{\mathrm{SC}}(C_{\mathsf{u}}(G)), \|.\|)$ is a Banach space as well. Thus, $i_{\mathrm{SC}}(C_{\mathsf{u}}(G))$ is closed in $C\big(\mathrm{SC}(G)\big)$.

Now, since $C_{\mathsf{u}}(G)$ and $i_{\mathrm{SC}}(C_{\mathsf{u}}(G))$ are isomorphic as Banach spaces, they are also isomorphic with their respective weak topologies. Therefore, for $f_n, f \in C_{\mathsf{u}}(G)$, we have

$$\{f_n\} \xrightarrow{\text{weakly}} f \quad\Longleftrightarrow\quad \{i_{\mathrm{SC}}(f_n)\} \xrightarrow[i_{\mathrm{SC}}(C_{\mathsf{u}}(G))]{\text{weakly in}} i_{\mathrm{SC}}(f).$$

Finally, since $i_{\mathrm{SC}}(C_{\mathsf{u}}(G))$ is closed in $C\big(\mathrm{SC}(G)\big)$, Lemma 4.4.4 implies

$$\{i_{\mathrm{SC}}(f_n)\} \xrightarrow[i_{\mathrm{SC}}(C_{\mathsf{u}}(G))]{\text{weakly in}} i_{\mathrm{SC}}(f) \quad\Longleftrightarrow\quad \{i_{\mathrm{SC}}(f_n)\} \xrightarrow[C(\mathrm{SC}(G))]{\text{weakly in}} i_{\mathrm{SC}}(f),$$

which completes the proof. □

[7] The theorem requires G to be a competely regular T_1-space, which is true for locally compact Hausdorff spaces.

Next, we show that, on compact spaces, weak convergence is equivalent to equi-boundedness and pointwise convergence.

Proposition 4.4.30. *Let X be a compact space. Then, for any sequence $\{f_n\} \subset C(X)$ and for $f \in C(X)$, the following statements are equivalent.*

(i) $\{f_n\} \xrightarrow{\text{weakly}} f$;

(ii) *The set $\{f_n\}_{n=1}^{\infty} \cup \{f\}$ is bounded in the sup-norm, and we have $\{f_n(x)\} \longrightarrow f(x)$ for all $x \in X$ as $n \to \infty$.*

Proof.
(i) $\Longrightarrow$ (ii): Since X is compact and the evaluation at x is a linear functional on $C(X)$, the pointwise convergence in claim (ii) is obvious. The boundedness is a consequence of the uniform boundedness principle (Theorem 4.4.8).

(ii) $\Longrightarrow$ (i): We use the fact that $C(X)' = C_{\mathsf{c}}(X)'$ with the weak-$*$ topology can be viewed as the space of all regular Borel measures with the vague topology on X; see the proof of the Krein–Šmulian theorem on page 209. To prove weak convergence, we thus only need to show that, for each measure μ on X, we have $\{\int f_n \,\mathrm{d}\mu\} \longrightarrow \int f \,\mathrm{d}\mu$. It is enough to do this for all positive measures μ and then, by taking real and imaginary parts, to do it for all real-valued f_n and f. But this is then just an exercise in Lebesgue's dominated convergence theorem. □

An immediate consequence of Theorem 4.4.29 and Proposition 4.4.30 is that weak convergence of sequences is preserved under multiplication.

Lemma 4.4.31. *Let $f_n, g_n, f, g \in C_{\mathsf{u}}(G)$ be so that*

$$\{f_n\} \xrightarrow{\text{weakly}} f \quad \text{and} \quad \{g_n\} \xrightarrow{\text{weakly}} g.$$

Then,

$$\{f_n g_n\} \xrightarrow{\text{weakly}} fg.$$

Proof. Using Theorem 4.4.29, from $\{f_n\} \xrightarrow{\text{weakly}} f$ we get

$$\{i_{\mathrm{SC}}(f_n)\} \xrightarrow{\text{weakly}} i_{\mathrm{SC}}(f).$$

Then, from Proposition 4.4.30, we find that $\{i_{\mathrm{SC}}(f_n)\}$ is equi-bounded with

$$\{i_{\mathrm{SC}}(f_n)\} \xrightarrow{\text{pointwise}} i_{\mathrm{SC}}(f).$$

In the same way, $\{i_{\mathrm{SC}}(g_n)\}$ is equi-bounded and

$$\{i_{\mathrm{SC}}(g_n)\} \xrightarrow{\text{pointwise}} i_{\mathrm{SC}}(g).$$

Then, $\{i_{\mathrm{SC}}(f_n)\, i_{\mathrm{SC}}(g_n)\}$ is equi-bounded and

$$\{i_{\mathrm{SC}}(f_n g_n)\} = \{i_{\mathrm{SC}}(f_n)\, i_{\mathrm{SC}}(g_n)\} \xrightarrow{\text{pointwise}} i_{\mathrm{SC}}(f)\, i_{\mathrm{SC}}(g) = i_{\mathrm{SC}}(fg).$$

Applying Proposition 4.4.30 again, $\{i_{\mathrm{SC}}(f_n g_n)\} \xrightarrow{\text{weakly}} i_{\mathrm{SC}}(fg)$, and then, by Theorem 4.4.29, $\{f_n g_n\} \xrightarrow{\text{weakly}} fg$. □

By combining Proposition 4.4.23, Theorem 4.4.29 and Proposition 4.4.30 we also get the following characterisation of weak almost periodicity.

Proposition 4.4.32. *Let $f \in C_{\mathsf{u}}(G)$. Then, $f \in \mathrm{WAP}(G)$ if and only if, for each sequence $\{t_n\}$ with $t_n \in G$, there exists a subsequence $\{t_{k_n}\}$ and some $g \in C_{\mathsf{u}}(G)$ such that*

$$\{i_{\mathrm{SC}}(t_{k_n}.f)\} \xrightarrow{\textit{pointwise}} i_{\mathrm{SC}}(g). \qquad \square$$

We can now prove the last part of Proposition 4.3.11.

Proof of Proposition 4.3.11 concluded. Consider part (v) and choose $f, g \in \mathrm{WAP}(G)$. Let $\{t_n\}$ be a sequence in G. By Proposition 4.4.23, there exists a subsequence $\{t_{k_n}\}$ and some $h_1 \in C_{\mathsf{u}}(G)$ such that

$$\{t_{k_n}.f\} \xrightarrow{\text{weakly}} h_1.$$

Since $g \in \mathrm{WAP}(G)$, Proposition 4.4.23 guarantees the existence of a subsequence $\{t_{\ell_n}\}$ of the sequence $\{t_{k_n}\}$ and some $h_2 \in C_{\mathsf{u}}(G)$ such that

$$\{t_{\ell_n}.g\} \xrightarrow{\text{weakly}} h_2.$$

Then, by Lemma 4.4.31, we have

$$\{t_{\ell_n}.(fg)\} \xrightarrow{\text{weakly}} h_1 h_2.$$

Proposition 4.4.23 now gives $fg \in \mathrm{WAP}(G)$.

Part (vi) is proved analogously. □

4.4.6. Almost invariant integrals and Eberlein's ergodic theorem

Definition 4.4.33. Let E be an LCTVS and let $\mathcal{R}$ be a semigroup of continuous linear operators on E. A *system of almost invariant integrals for $\mathcal{R}$* is a net $\{S_\alpha\}$ of mappings of E into itself with the following properties.

(i) Each $S_\alpha \colon E \longrightarrow E$ is linear;

(ii) For all α and for all $f \in E$, we have $S_\alpha f \in \mathcal{C}_f(\mathcal{R})$ (see our notation in Eq. (4.4.5));

(iii) The set $\{S_\alpha\}$ is equicontinuous;

(iv) For all $f \in E$ and $R \in \mathcal{R}$, one has
   (a) $\lim_\alpha (RS_\alpha f - S_\alpha f) = 0$,
   (b) $\lim_\alpha (S_\alpha R f - S_\alpha f) = 0$.

The meaning of equicontinuity in property (iii) is the following. To say that S_α is continuous is to say that, for each semi-norm ϕ defining the topological structure of the LCTVS E, there is a positive constant c_α for which $\|S_\alpha f\|_\phi \leqslant c_\alpha \|f\|_\phi$ for all $f \in E$. The family of operators is equicontinuous if this constant can be taken to be the same for the entire family.

Example 4.4.34. The motivating example for this definition is $C_{\mathsf{u}}(G)$ with the system of operators $S_n \colon C_{\mathsf{u}}(G) \longrightarrow C_{\mathsf{u}}(G)$, where $S_n(f)$ is the function defined by

$$x \longmapsto \big(S_n(f)\big)(x) := \frac{1}{\theta_G(A_n)} \int_{A_n} T_{-x} f \, \mathrm{d}\theta_G,$$

relative to some van Hove sequence $\{A_n\}$; compare Eq. (4.1.4). This is a system of almost invariant integrals for the group of operators $\{T_x : x \in G\}$, via Proposition 4.5.2 below. ◊

Remark 4.4.35.

(1) An LCAG G that admits a system of almost invariant integrals is called *amenable*.

(2) For all our applications of systems of almost invariant integrals, we shall have $RS_\alpha = S_\alpha R$ for all $R \in \mathcal{R}$, whereby (iv)(b) becomes redundant.

(3) If $\{\mathcal{R}\}$ is equicontinuous, then (iii) follows from (ii). This can be seen as follows: For $f \in E$ and any α, assumption (ii) of Definition 4.4.33 says that $S_\alpha f \in \mathcal{C}_f$. Also, any point of $\mathcal{C}_f$ is a limit of finite convex sums of the form $\sum_i a_i R_i f$. Then, for all α and for each of the semi-norms $\|.\|_\phi$ defining the topology of E,

$$\|S_\alpha f\|_\phi \leqslant \sup_{\{a_i\}} \sum_i a_i \|R_i f\|_\phi \leqslant \sup_{\{a_i\}} \sum_i a_i c \, \|f\|_\phi \leqslant c \|f\|_\phi$$

for some constant c that depends on the semi-norm and the assumed equicontinuity of the family of operators $\mathcal{R}$. The supremum is taken over all finite convex combinations.

(4) If E is a Banach space, parts (iii) and (iv) of Definition 4.4.33 take the following equivalent forms.

(iii′) There exists an m so that $\|S_\alpha\| \leqslant m$ for all α;

(iv′) $\lim_\alpha (RS_\alpha - S_\alpha) = \lim_\alpha (S_\alpha R - S_\alpha) = 0$ in the space of continuous linear operators on E. ◊

Theorem 4.4.36 (Eberlein's ergodic theorem [15, Thm. 3.1])**.** *Let the space E be an LCTVS, let $\mathcal{R}$ be a semigroup with a system $\{S_\alpha\}$ of almost invariant integrals, and let $f, g \in E$. Then, the following statements are equivalent,*

(i) *$g \in \mathcal{C}_f(\mathcal{R})$ and g is $\mathcal{R}$-invariant;*

(ii) $g = \lim_\alpha(S_\alpha f)$ *in* E*, where the limit is in the strong topology of* E*;*

(iii) $g = \text{w-}\lim_\alpha(S_\alpha f)$*;*

(iv) g *is a weak cluster point of* $\{S_\alpha f\}$*.*

PROOF. The implications (ii) $\Longrightarrow$ (iii) $\Longrightarrow$ (iv) are clear, so in order to complete the proof, we will show (iv) $\Longrightarrow$ (i) $\Longrightarrow$ (ii).

(i) $\Longrightarrow$ (ii). Let U be an open neighbourhood of 0 in E and let $V = -V$ be taken so that $V - V \subseteq U$. Since $\{S_\alpha\}$ is equicontinuous, there exists an open neighbourhood W of 0 so that $S_\alpha(W) \subseteq V$ for all α.

Since $g \in \mathcal{C}_f$, there exists an $r^* \in \mathcal{R}^*$ so that $g - r^*f \in W$, compare Eq. (4.4.5), hence

$$S_\alpha g - S_\alpha(r^*f) \in V \tag{4.4.10}$$

for all α. Since $\lim_\alpha\big(S_\alpha(r^*f) - S_\alpha f\big) = 0$, there exists an α_0 so that, for all $\alpha > \alpha_0$, we have

$$S_\alpha(r^*f) - S_\alpha f \in V. \tag{4.4.11}$$

Putting Eqs. (4.4.10) and (4.4.11) together, we get $S_\alpha g - S_\alpha f \in U$. However, $S_\alpha g \in \mathcal{C}_g$ and g is $\mathcal{R}$-invariant, so $\mathcal{C}_g = \{g\}$ and $S_\alpha g = g$. So, for all $\alpha > \alpha_0$, we have $g - S_\alpha f \in U$, and this shows that $\{S_\alpha f\}$ converges to g.

(iv) $\Longrightarrow$ (i). Let $R \in \mathcal{R}$, $\varepsilon > 0$, and let $\phi \in E'$ be arbitrary. Define $\phi' \in E'$ by $\phi'(f) = \phi(Rf)$. Since $\lim_\alpha(RS_\alpha f - S_\alpha f) = 0$, there exists an α_0 so that, for all $\alpha > \alpha_0$, we have

$$|\phi(RS_\alpha f - S_\alpha f)| < \varepsilon. \tag{4.4.12}$$

Let U be the open set defined by ϕ, ϕ' and ε in the weak topology, that is

$$U := \big\{f \in E : |\phi(f)| < \varepsilon, |\phi'(f)| < \varepsilon\big\}.$$

Since g is a weak cluster point of $\{S_\alpha f\}$, there exists an $\alpha_1 > \alpha_0$ so that $S_{\alpha_1} f - g \in U$. Thus, we get

$$\begin{aligned} \big|\phi(RS_{\alpha_1} f) - \phi(S_{\alpha_1} f)\big| &< \varepsilon, \\ \big|\phi(S_{\alpha_1} f) - \phi(g)\big| &< \varepsilon, \\ \big|\phi(RS_{\alpha_1} f) - \phi(Rg)\big| &< \varepsilon. \end{aligned}$$

Adding these three relations gives $|\phi(Rg - g)| < 3\varepsilon$. Since $\varepsilon > 0$ is arbitrary, we get $\phi(Rg - g) = 0$. As $\phi \in E'$ is arbitrary, Theorem 4.4.3 (Hahn–Banach) gives $Rg = g$. Finally, since $R \in \mathcal{R}$ is also arbitrary, g is $\mathcal{R}$-invariant.

Also, since g is a weak cluster point of $\{S_\alpha f\} \subset \mathcal{C}_f$ and $\mathcal{C}_f$ is weakly closed by Theorem 4.4.10, we get $g \in \mathcal{C}_f$. □

Remark 4.4.37.

(1) The equivalence (i) $\iff$ (ii) shows that there exists at most one $\mathcal{R}$-invariant element in $\mathcal{C}_f$.

(2) The equivalence (i) $\iff$ (ii) also shows that, if the $\lim_\alpha(S_\alpha f)$ exists, it is independent of the choice of the system of almost invariant integrals.

(3) If $\mathcal{C}_f(\mathcal{R})$ is weakly compact, every net $\{S_\alpha f\}_\alpha$ has a weak cluster point g, and all four statements about the function g in Theorem 4.4.36 are true. $\Diamond$

4.5. Means

Let G be an LCAG. In this section, we begin to study the mean, already introduced in Definition 4.1.6. Functions for which the mean exists are called *amenable*. Applying the results of Section 4.4 to the Banach space $C_{\mathsf{u}}(G)$, we shall find that the elements of $\mathrm{WAP}(G)$ are amenable functions. Let us recall a concept that is closely related to the definition of a van Hove sequence.

Definition 4.5.1. Let G be an LCAG. A sequence $\{A_n\}$ of compact sets $A_n \subseteq G$, with $0 < \theta_G(A_n) < \infty$ for all n, is called a *Følner sequence* if

$$\lim_{n\to\infty} \frac{\theta_G\big((g + A_n)\triangle A_n\big)}{\theta_G(A_n)} \,=\, 0$$

holds for all $g \in G$. Here, $\triangle$ denotes the symmetric difference of sets, as defined by $A\triangle B = (A \setminus B) \cup (B \setminus A)$.

Since $A_n\triangle(g+A_n) \subseteq \partial^{\{0,g\}}A_n$ for every $g \in G$, any van Hove sequence is a Følner sequence; compare Eq. (4.1.3) on page 179. Note that the converse is generally not true; see [AO1, Rem. 2.5] and the discussion in [3] for details.

Proposition 4.5.2. *Let $\{A_n\}$ be a Følner sequence in the LCAG G, and let $S_n\colon C_{\mathsf{u}}(G) \longrightarrow C_{\mathsf{u}}(G)$ be the mapping $f \mapsto S_n(f)$ of Example* 4.4.34*, where*

$$\big(S_n(f)\big)(x) \,=\, \frac{1}{\theta_G(A_n)} \int_{A_n} f(x+t)\,\mathrm{d}t.$$

Then indeed, each S_n maps into $C_{\mathsf{u}}(G)$, and $\{S_n\}$ defines a system of almost invariant integrals for the G-action on $C_{\mathsf{u}}(G)$ (that is, we are taking the group of operators $\mathcal{G} := \{T_x : x \in G\}$).

In particular, if $\{A_n\}$ is a van Hove sequence, $\{S_n\}$ is a system of almost invariant integrals.

Proof. It is easy to see that each S_n is linear (property (i) of Definition 4.4.33 for a system of almost invariant integrals) and that, for any f

and x, it has the property

$$\big|\big(S_n(f)\big)(x)\big| \leqslant \|f\|_\infty. \tag{4.5.1}$$

This shows (iii). It also shows that $S_n(f)$ is a bounded function, and, since $\big|\big(S_n(f)\big)(x) - \big(S_n(f)\big)(y)\big| \leqslant \|f - T_{y-x}f\|_\infty$, one has $S_n(f) \in C_{\mathsf{u}}(G)$.

Let us now prove properties (ii) and (iv) of a system of almost invariant integrals.

To show property (ii), let $f \in C_{\mathsf{u}}(G)$ and fix some $\varepsilon > 0$. Then, there exists an open neighbourhood U of 0 so that, for all x, y with $x - y \in U$, we have $|f(x) - f(y)| < \varepsilon$. Fix any n. Since A_n is compact, we can cover it by finitely many translates of U. By refining these sets, we can arrange the setting so that there are measurable, pairwise disjoint Borel sets V_i and translations $t_i \in G$ for which

$$A_n \,=\, \bigcup_{i=1}^{m} V_i \quad \text{and} \quad V_i \,\subseteq\, t_i + U.$$

Let[8]

$$T_n^* \,:=\, \sum_{i=1}^{m} \frac{\theta_G(V_i)}{\theta_G(A_n)}\, T_{t_i} \,\in\, \mathcal{G}^*.$$

Then, for all $t \in G$,

$$\begin{aligned}
\big|(T_n^* - S_n)(f)(t)\big| \,&=\, \left| \sum_{i=1}^{m} \frac{\theta_G(V_i)}{\theta_G(A_n)}\, f(t+t_i) - \frac{\int_{A_n} f(t+s)\,\mathrm{d}s}{\theta_G(A_n)} \right| \\
&=\, \frac{1}{\theta_G(A_n)} \left| \sum_{i=1}^{m} \left(\int_{V_i} f(t+t_i)\,\mathrm{d}s - \int_{V_i} f(t+s)\,\mathrm{d}s \right) \right| \\
&\leqslant \frac{1}{\theta_G(A_n)} \sum_{i=1}^{m} \int_{V_i} \big| f(t+t_i) - f(t+s) \big|\,\mathrm{d}s.
\end{aligned}$$

Now, $(t+s)-(t+t_i) = s - t_i \in -t_i + V_i \subseteq U$, thus $|f(t+t_i) - f(t+s)| < \varepsilon$, so $|(T_n^* - S_n)(f)(t)| < \varepsilon$. Hence,

$$\|T_n^*(f) - S_n(f)\|_\infty \,\leqslant\, \varepsilon. \tag{4.5.2}$$

This shows that $S_n(f) \in \overline{\mathcal{G}^* f} = \mathcal{C}_f$ in $C_{\mathsf{u}}(G)$, as required.

Finally, let us prove property (iv). Since

$$\begin{aligned}
S_n(T_y f)(x) \,&=\, \frac{\int_{A_n} T_y f(x+t)\,\mathrm{d}t}{\theta_G(A_n)} \,=\, \frac{\int_{A_n} f(x-y+t)\,\mathrm{d}t}{\theta_G(A_n)} \\
&=\, S_n(f)(x-y) \,=\, T_y(S_n f)(x),
\end{aligned}$$

[8]For the definition of $\mathcal{G}^*$, see Eq. (4.4.5) and the following text on page 197.

it is enough to prove only (iv)(b). Let $y \in G$ and let $\triangle$ again denote the symmetric difference. Then,

$$\begin{aligned}
\big|\big(S_n(f)\big)(x) - \big(S_n(T_y f)\big)(x)\big| \;&=\; \left| \frac{\int_{A_n} f(x+t)\,\mathrm{d}t}{\theta_G(A_n)} - \frac{\int_{A_n} T_y f(x+t)\,\mathrm{d}t}{\theta_G(A_n)} \right| \\
&=\; \frac{1}{\theta_G(A_n)} \left| \int_{A_n} f(x+t)\,\mathrm{d}t - \int_{A_n} f(x-y+t)\,\mathrm{d}t \right| \\
&=\; \frac{1}{\theta_G(A_n)} \left| \int_{A_n} f(x+t)\,\mathrm{d}t - \int_{y+A_n} f(x+t)\,\mathrm{d}t \right| \\
&=\; \frac{1}{\theta_G(A_n)} \left| \int_{A_n \,\triangle\, (y+A_n)} f(x+t)\,\mathrm{d}t \right| \\
&\leqslant\; \frac{\|f\|_\infty\, \theta_G(A_n \triangle (y+A_n))}{\theta_G(A_n)} \;\xrightarrow{\;n\to\infty\;}\; 0,
\end{aligned}$$

the last step due to the Følner property of the sequence $\{A_n\}$. The claim on the van Hove sequences is then clear. □

Corollary 4.5.3. *The translation action of G on $C_{\mathsf{u}}(G)$ admits a system of almost invariant integrals.* □

Remark 4.5.4. Note that, in the proof of part (ii) of Proposition 4.5.2, the operator T_n^* that makes Eq. (4.5.2) work depends only on the neighbourhood U for which $x - y \in U \implies |f(x) - f(y)| < \varepsilon$. Thus, if $\{h_s\}$ is an equicontinuous family of functions from $C_{\mathsf{u}}(G)$, we can arrange to have $\|T_n^* h_s - S_n h_s\|_\infty < \varepsilon$ for all h_s simultaneously. We will use this remark in Proposition 4.7.4. ♢

Applying Theorem 4.4.36 to Proposition 4.5.2, we see that, if $f \in C_{\mathsf{u}}(G)$ and $g = \text{w-lim}_{n\to\infty} S_n(f)$ exists in $C_{\mathsf{u}}(G)$, then $g \in \mathcal{C}_f$ and g is G-invariant, that is, $T_x g = g$ for all $x \in G$. Thus, g is the constant function $M(f)\,1_G$ for some complex number $M(f)$.

Definition 4.5.5. A function $f \in C_{\mathsf{u}}(G)$ is *amenable* if the limit

$$\lim_{n\to\infty} \big(S_n(f)\big)(x) \;=\; \lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \int_{A_n} f(x+t)\,\mathrm{d}\theta_G(t)$$

exists uniformly in $x \in G$. In this case, the limit is a constant function, $M(f)\,1_G$, which is called the *mean* of f.

Of course, this definition implies that we can define $M(f)$ simply as

$$M(f) \;=\; \lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \int_{A_n} f(t)\,\mathrm{d}\theta_G(t),$$

and see immediately that it is unaltered by a translation action on f; compare Proposition 4.5.9(iv).

Theorem 4.4.36 in conjunction with the above discussion now gives the following result.

Proposition 4.5.6. *Assume the context of Proposition* 4.5.2. *For two functions $f, g \in C_{\mathsf{u}}(G)$, the following statements are equivalent,*

(i) *$g \in \mathcal{C}_f$ and g is constant;*
(ii) *f is amenable and $g = M(f)\, 1_G$;*
(iii) *$\{S_n f\}$ converges strongly to g;*
(iv) *$\{S_n f\}$ converges weakly to g;*
(v) *g is a weak cluster point of $\{S_n f\}$.* □

Remark 4.5.7. From statement (i), we see that the notion of amenability, and then the resulting mean, are independent of the choice of the Følner sequence $\{A_n\}$. ◊

Example 4.5.8. Let us emphasise here that the uniformity of the limit in Definition 4.5.5 is crucial. Without it, the amenability and the mean of the function would depend on the choice of the Følner sequence and statement (ii) in Proposition 4.5.6 would become weaker than the others.

For example, consider the continuous function

$$f(x) := \begin{cases} 0, & \text{if } x \leqslant 0, \\ x, & \text{if } 0 < x < 1, \\ 1, & \text{if } x \geqslant 1. \end{cases}$$

Then, one has

$$\lim_{n\to\infty} \frac{1}{n} \int_0^n f(x+t)\, \mathrm{d}t \;=\; 1,$$

$$\lim_{n\to\infty} \frac{1}{n} \int_{-n}^0 f(x+t)\, \mathrm{d}t \;=\; 0,$$

$$\lim_{n\to\infty} \frac{1}{2n} \int_{-n}^n f(x+t)\, \mathrm{d}t \;=\; \frac{1}{2}.$$

All these limits exist pointwise, but not uniformly in t. Indeed, were any of the limits uniform, f would be amenable, and hence all the limits would be the same. Also, for this function, the mean does not exist for the van Hove sequence defined by $A_n = \big[(-1)^n n - n, n\big]$. ◊

Proposition 4.5.9 ([15, Thm. 14.1])**.** *Every $f \in \mathrm{WAP}(G)$ is amenable. The mean $M\colon \mathrm{WAP}(G) \longrightarrow \mathbb{C}$ has the following properties.*

(i) *M is $\mathbb{C}$-linear;*

(ii) $M(1_G) = 1$;

(iii) $f \geqslant 0 \implies M(f) \geqslant 0$;

(iv) $M(T_y f) = M(f)$ *for all* $y \in G$;

(v) $|M(f)| \leqslant M(|f|) \leqslant \|f\|_\infty$ (*in particular,* $M \in \mathrm{WAP}(G)'$);

(vi) $M(f^\dagger) = M(f)$ *and* $M(\overline{f}) = \overline{M(f)} = M(\widetilde{f})$;

(vii) *If* $p, q \geqslant 1$ *with* $\frac{1}{p} + \frac{1}{q} = 1$, *and if* $f, g \in \mathrm{WAP}(G)$, *one has*

$$\big|M(fg)\big| \leqslant \big[M(|f|^p)\big]^{\frac{1}{p}} \big[M(|g|^q)\big]^{\frac{1}{q}}.$$

Moreover, any linear mapping $L : \mathrm{WAP}(G) \longrightarrow \mathbb{C}$ *which verifies* (i)–(iv) *must coincide with* M.

Proof. Let $f \in \mathrm{WAP}(G)$. Then, $\mathcal{C}_f$ is weakly compact by Corollary 4.4.28, and then weakly sequentially compact by Theorem 4.4.19. Hence, $\{S_n(f)\}$ has a weak cluster point, and f is amenable by Proposition 4.5.6.

Properties (i)–(iii) and (v)–(vi) follow immediately from the corresponding properties of the integral, using the Følner sequence $\{-A_n\}$ for $\widetilde{f}$ and $f^\dagger$. Property (iv) follows from the fact that $M(f)\,1_G$ is the only constant function in $\mathcal{C}_f$ in conjunction with the fact that $M(T_y f)\,1_G$ is a constant function in $\mathcal{C}_{T_y f} \subseteq \mathcal{C}_f$.

Let us prove (vii). Since $f, g \in \mathrm{WAP}(G)$, we get $fg, |f|^p, |g|^q \in \mathrm{WAP}(G)$ by Proposition 4.3.11, so all the means make sense. Using Hölder's inequality, one finds

$$\begin{aligned}
\big|M(fg)\big| &= \left|\lim_n \frac{\int_{A_n} f(t)g(t)\,\mathrm{d}t}{\theta_G(A_n)}\right| = \lim_n \frac{\left|\int_{A_n} f(t)g(t)\,\mathrm{d}t\right|}{\theta_G(A_n)} \\
&\leqslant \lim_n \frac{\big[\int_{A_n} |f(t)|^p\,\mathrm{d}t\big]^{\frac{1}{p}} \big[\int_{A_n} |g(t)|^q\,\mathrm{d}t\big]^{\frac{1}{q}}}{[\theta_G(A_n)]^{\frac{1}{p}}\,[\theta_G(A_n)]^{\frac{1}{q}}} \\
&= \lim_n \frac{\big[\int_{A_n} |f(t)|^p\,\mathrm{d}t\big]^{\frac{1}{p}}}{[\theta_G(A_n)]^{\frac{1}{p}}} \lim_n \frac{\big[\int_{A_n} |g(t)|^q\,\mathrm{d}t\big]^{\frac{1}{q}}}{[\theta_G(A_n)]^{\frac{1}{q}}} \\
&= \lim_n \left[\frac{\int_{A_n} |f(t)|^p\,\mathrm{d}t}{\theta_G(A_n)}\right]^{\frac{1}{p}} \lim_n \left[\frac{\int_{A_n} |g(t)|^q\,\mathrm{d}t}{\theta_G(A_n)}\right]^{\frac{1}{q}} \\
&= \big[M(|f|^p)\big]^{\frac{1}{p}} \big[M(|g|^q)\big]^{\frac{1}{q}}.
\end{aligned}$$

If L is a linear map which verifies (i)–(iv), then L is constant on $\mathcal{G}^* f$ by (i) and (iv). Let $f \in \mathrm{WAP}(G)$ be real-valued. Since $-\|f\|_\infty 1_G \leqslant f \leqslant \|f\|_\infty 1_G$, we obtain from (iii) that

$$-\|f\|_\infty \leqslant L(f) \leqslant \|f\|_\infty.$$

Since $\mathrm{WAP}(G)$ is linear and closed under complex conjugation, we deduce that $\mathrm{Re}(g) = (g+\overline{g})/2$ and $\mathrm{Im}(g) = (g+\overline{g})/2\mathrm{i}$ are real-valued weakly almost periodic functions, for any $g \in \mathrm{WAP}(G)$. Thus,

$$\begin{aligned} |L(g)| \;&=\; |L(\mathrm{Re}(g)) + \mathrm{i}\, L(\mathrm{Im}(g))| \;\leqslant\; |L(\mathrm{Re}(g))| + |L(\mathrm{Im}(g))| \\ &\leqslant\; \|\mathrm{Re}(g)\|_\infty + \|\mathrm{Im}(g)\|_\infty \;\leqslant\; 2\|g\|_\infty, \end{aligned}$$

and hence L is continuous on $\mathrm{WAP}(G)$. Since L is constant on $\mathcal{G}^* f$ and continuous, L is constant on C_f. So, since f and $M(f)\,1_G$ are in C_f, we obtain the relation

$$L(f) \;=\; L\big(M(f)\,1_G\big) \;=\; M(f)\,L(1_G) \;=\; M(f),$$

where property (ii) for L was used. Thus, $L = M$ on real-valued functions, and the rest follows from properties (i) and (ii). □

Proposition 4.5.10. *Let $f \in \mathrm{SAP}(G)$ (resp. $\mathrm{WAP}(G)$) and let $g \in C_{\mathsf{c}}(G)$. Then, $f * g \in \mathrm{SAP}(G)$ (resp. $\mathrm{WAP}(G)$), and it is amenable with*

$$M(f * g) \;=\; M(f) \int_G g \,\mathrm{d}\theta_G.$$

Proof. Given $g \in C_{\mathsf{c}}(G)$, the mapping $f \mapsto f * g$ of $C_{\mathsf{u}}(G)$ to itself is continuous (in the strong topology). It is also a G-map. Thus, if $G.f$ has compact closure in $C_{\mathsf{u}}(G)$, so does $G.(f * g)$, and it then follows from the definition of $\mathrm{SAP}(G)$ that $\mathrm{SAP}(G)$ maps into itself. Also, by Lemma 4.4.2, strong continuity implies weak continuity, and we see that $\mathrm{WAP}(G)$ maps into itself. It remains to prove the statement on the mean, which follows from

$$\begin{aligned} M(f*g) &= \lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \int_{A_n} \big(f*g\big)(x+t)\,\mathrm{d}t \\ &= \lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \int_{A_n} \int_G f(x+t-u)\, g(u)\,\mathrm{d}u\,\mathrm{d}t \\ &= \int_G \left(\lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \int_{A_n} f(x+t-u)\,\mathrm{d}t \right) g(u)\,\mathrm{d}u \\ &= M(f) \int_G g(t)\,\mathrm{d}t \;=\; M(f)\,\theta_G(g), \end{aligned}$$

where dominated convergence is used to rearrange limits and integrals. □

The next result shows that the mean behaves nicely when we move from functions of one variable to functions of two variables.

$$M_s(f)\colon \quad M_s(f)(t) \;=\; \lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \int_{A_n} f(s,t)\,\mathrm{d}\theta_G(s),$$

$$M_t(f)\colon \quad M_t(f)(s) \;=\; \lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \int_{A_n} f(s,t)\,\mathrm{d}\theta_G(t).$$

These functions are termed the mean of f with t fixed and the mean of f with s fixed, respectively.

Proposition 4.5.11 ([15, Thm. 14.2])**.** *If $f \in \mathrm{WAP}(G)$, then g and h defined by $g(t,s) = f(t+s)$ and $h(t,s) = f(t)$ are in $\mathrm{WAP}(G\times G)$. In the other direction, if $f \in \mathrm{WAP}(G\times G)$, then $f(s,t)$ is weakly almost periodic both as a function of s with t fixed and as a function of t with s fixed. Furthermore, the means $M_s(f)$ and $M_t(f)$ — as functions of one variable — are weakly almost periodic, and*

$$M_s(M_t(f(s,t))) \;=\; M_t(M_s(f(s,t))) \;=\; M_{(s,t)}(f(s,t)).$$

Proof. The mapping $f \mapsto g$ is a continuous and norm-preserving linear mapping

$$\beta\colon \mathrm{WAP}(G) \;\longrightarrow\; C_{\mathsf{u}}(G\times G),$$

and, for all $x, y \in G$,

$$\begin{aligned}\big(T_{(y,x)}g\big)(t,s) \;&=\; g(-y+t,-x+s) \;=\; f(-(y+x)+t+s)\\ &=\; \big(T_{y+x}\big)f(t+s) \;=\; \big(\beta(T_{y+x}f)\big)(t,s).\end{aligned}$$

Thus, we have $\beta(G.f) \supseteq (G\times G).g$. Since $\overline{G.f}$ is weakly compact, so also are $\beta\big(\overline{G.f}\big) = \overline{\beta(G.f)}$ and $\overline{(G\times G).g}$, thus $g \in \mathrm{WAP}(G\times G)$. The argument for h is similar.

We next show that, whenever $f \in \mathrm{WAP}(G\times G)$, the mean satisfies $M_s(f) \in \mathrm{WAP}(G)$. First, we demonstrate that $M_s(f) \in C_{\mathsf{u}}(G)$ and that

$$M_s\colon \mathrm{WAP}(G\times G) \longrightarrow C_{\mathsf{u}}(G)$$

is a continuous mapping.

It is obvious that M_s is linear and that $\|M_s(f)\|_\infty \leqslant \|f\|_\infty$. Let $\varepsilon > 0$. Since f is uniformly continuous, there exists a neighbourhood of $(0,0)$ in $G\times G$ of type $U\times V$ so that $\|f - T_{(x,y)}f\|_\infty < \varepsilon$ for all $(x,y) \in U\times V$. Let $y \in V$. Then, for all $t \in G$,

$$\big|M_s(f)(t) - T_y(M_s(f))(t)\big| \;=\; \big|M_s(f(s,t)) - M_s(f(s,t-y))\big|.$$

As $|f(s,t) - f(s,t-y)| \leqslant \big\|f - T_{(0,y)}f\big\|_\infty$, we have

$$\big|M_s(f)(t) - T_y(M_s(f))(t)\big| \;\leqslant\; \big\|f - T_{(0,y)}f\big\|_\infty < \varepsilon,$$

which proves $M_s(f) \in C_{\mathsf{u}}(G)$.

Since $\|M_s(h)\|_\infty = \|M_s(h(s,\cdot))\|_\infty \leqslant \|h\|_\infty$ for all $h \in \mathrm{WAP}(G\times G)$, we see that M_s is strongly continuous. It is then also weakly continuous by Lemma 4.4.2. Thus, M_s takes weakly compact sets into weakly compact sets. So, if f is weakly almost periodic, then so is $M_s(f)$, which completes the argument and shows that $M_s(f(s,t)) \in \mathrm{WAP}(G)$. The proof for the inclusion $M_t(f(s,t)) \in \mathrm{WAP}(G)$ works in the same way.

It is straightforward to see that the composition

$$\mathrm{WAP}(G\times G) \xrightarrow{M_s} \mathrm{WAP}(G) \xrightarrow{M_t} \mathbb{C}$$

satisfies properties (i)–(iv) of Proposition 4.5.9 for $G\times G$, and so must be the same as $M_{(s,t)}$. □

We complete this section by pointing out a result due to Argabright which shows that there are many sets of test functions through which the mean can be calculated. As the result is not relevant to the rest of the paper, we skip the proof and refer the reader to [2] instead.

Lemma 4.5.12 ([2])**.** *Let $\{f_\alpha\}_\alpha$ be a net of functions in $L^1(G)$ such that*

(i) *for all α, we have $\int_G f_\alpha(t)\,\mathrm{d}\theta_G(t) = 1$;*

(ii) *for all $x \in G$, we have $\lim_\alpha \|f_\alpha - T_x f_\alpha\|_1 = 0$.*

Then, for all $f \in \mathrm{WAP}(G)$, we have

$$M(f) = \lim_\alpha \int_G f(t)\, f_\alpha(t)\,\mathrm{d}\theta_G(t). \qquad \square$$

4.6. The Eberlein convolution

Definition 4.6.1. The *Eberlein convolution* of two weakly almost periodic functions f and g is the function $f \star g$, where

$$\bigl(f\star g\bigr)(t) := M_s\bigl(f(t-s)g(s)\bigr) = M_s\bigl(f(s)g(t-s)\bigr).$$

Remark 4.6.2. The existence of the mean comes from the closure of the space $\mathrm{WAP}(G)$ under multiplication and translations, while the equivalence of the two definitions follows from the invariance of the mean M under translations and reflections. Since M is continuous by Theorem 4.5.9(v), the Eberlein convolution is continuous in both its variables. From Proposition 4.5.11, it is easy to show that

$$f\star(g\star h) = (f\star g)\star h$$

holds for all $f, g, h \in \mathrm{WAP}(G)$. Since $f\star g = g\star f$, the Eberlein convolution is thus both associative and commutative. ♢

Theorem 4.6.3 ([15, Thm. 15.1])**.** *If $f, g \in \mathrm{WAP}(G)$, then $f\star g \in \mathrm{SAP}(G)$.*

PROOF. We need to prove that $\mathcal{C}_{f\star g}$ is compact in the strong topology. For this, it suffices to show that it is sequentially compact. Let $\{x_n\}$ be a sequence in G. We prove that $\bigl\{T_{x_n}(f\star g)\bigr\}$ has a convergent subsequence in the strong topology. Observe that

$$\begin{aligned} T_{x_n}\bigl(f\star g\bigr)(t) \,&=\, \bigl(f\star g\bigr)(-x_n+t) \,=\, M_s\bigl(f(s)\,g(-x_n+t-s)\bigr) \\ &=\, M_s\bigl((T_{x_n}f)(s)\,g(t-s)\bigr). \end{aligned}$$

Since f is weakly almost periodic, there exists a subsequence $\{y_m\}$ of $\{x_n\}$ and a function $h\in C_{\mathsf{u}}(G)$ so that

$$\operatorname*{w-lim}_m T_{y_m}(f) \,=\, h.$$

We note that, since $T_{y_m}(f)\in\mathcal{C}_f$ and since $\mathcal{C}_f$ is weakly compact by Corollary 4.4.28, we have $h\in\mathcal{C}_f$. It follows that $\mathcal{C}_h\subseteq\mathcal{C}_f$ is also weakly compact, and hence $h\in\mathrm{WAP}(G)$. Using Proposition 4.5.9(vii), we have, for all $t\in G$,

$$\begin{aligned} \bigl|T_{y_m}\bigl(f\star g\bigr)(t)-\bigl(h\star g\bigr)(t)\bigr|^2 \,&=\, \bigl|(f\star g)(-y_m+t)-M_s\bigl(h(s)g(t-s)\bigr)\bigr|^2 \\ &=\, \bigl|M_s\bigl(T_{y_m}(f)(s)\,g(t-s)\bigr)-M_s\bigl(h(s)g(t-s)\bigr)\bigr|^2 \\ &=\, \bigl|M_s\bigl((T_{y_m}(f)(s)-h(s))g(t-s)\bigr)\bigr|^2 \qquad (4.6.1) \\ &\leqslant\, M_s\bigl(|T_{y_m}(f)(s)-h(s)|^2\bigr)\,M_s\bigl(|g(t-s)|^2\bigr) \\ &\leqslant\, \|g\|_\infty^2\,M\bigl(|T_{y_m}(f)-h|^2\bigr). \end{aligned}$$

Since we know that $\text{w-lim}_m\,|T_{y_m}(f)-h|=0$, Lemma 4.4.31 tells us that

$$\operatorname*{w-lim}_m |T_{y_m}(f)-h|^2 \,=\, 0.$$

Now, using that M is a continuous linear functional on $\mathrm{WAP}(G)$, we obtain $\lim_m M\bigl(|T_{y_m}(f)-h|^2\bigr)=0$. Along with Eq. (4.6.1), this shows that we have $\bigl\{T_{y_m}(f\star g)\bigr\}\longrightarrow h\star g$ in the sup-norm, which completes the proof. □

Since $\mathrm{WAP}(G)$ is closed under multiplication by Proposition 4.3.11, it is an immediate consequence of Proposition 4.5.9 that $\mathrm{WAP}(G)$ becomes a positive semi-definite inner product space with respect to the inner product

$$\langle g|f\rangle \,:=\, M(f\overline{g}), \qquad (4.6.2)$$

where we again use the convention that the inner product is linear in the second argument. This convention has its advantage in formal calculations with Fourier expansions in Dirac's formalism; compare [37].

Lemma 4.6.4. *Let $\chi\in\widehat{G}$ be non-trivial. Then, $M(\chi)=0$. In particular, $\widehat{G}$ is an orthonormal set with respect to $\langle\cdot|\cdot\rangle$ from Eq.* (4.6.2).

PROOF. Since χ is periodic, it is strongly almost periodic and thus weakly almost periodic; see also Example 4.3.1. Since χ is not identically 1, there exists an x with $\chi(x) \neq 1$. Hence

$$M(\chi) \,=\, M(T_x\chi) \,=\, \chi(x)M(\chi).$$

Thus, $M(\chi)(1-\chi(x)) = 0$ and $M(\chi) = 0$.

If $\chi \neq \psi$ are two characters, $\overline{\chi}\psi$ is another non-trivial character, whence $\langle\chi|\psi\rangle = M(\overline{\chi}\psi) = 0$ shows the claimed orthogonality. Finally, the normalisation follows from $M(1) = 1$. □

Definition 4.6.5. For $f \in \mathrm{WAP}(G)$ and $\chi \in \widehat{G}$, we define

$$a_f(\chi) \,:=\, \langle\chi|f\rangle \,=\, M(f\overline{\chi})$$

to be the *Fourier–Bohr coefficient* of f.

For an $f \in \mathrm{WAP}(G)$, we will look at the formal Fourier series

$$f \,=\, |f\rangle \,\sim\, \sum_{\chi\in\widehat{G}} |\chi\rangle\langle\chi|f\rangle \,=\, \sum_{\chi\in\widehat{G}} a_f(\chi)\,\chi.$$

Here, we have used a bit of Dirac notation, in terms of which we also have the formal completeness relation $\sum_{\chi\in\widehat{G}} |\chi\rangle\langle\chi| = \mathbb{1}$.

Lemma 4.6.6 ([15, Lemma 15.1])**.** *Let $f \in \mathrm{WAP}(G)$ and let $\chi_1, \dots, \chi_n \in \widehat{G}$ be distinct. Then, one has*

$$M\Bigl(\Bigl|f - \sum_{i=1}^{n} a_f(\chi_i)\,\chi_i\Bigr|^2\Bigr) \,=\, M\bigl(|f|^2\bigr) - \sum_{i=1}^{n} \bigl|a_f(\chi_i)\bigr|^2.$$

In particular, we get Bessel's inequality

$$\sum_{\chi\in\widehat{G}} \bigl|a_f(\chi)\bigr|^2 \,\leqslant\, M\bigl(|f|^2\bigr) \,<\, \infty.$$

PROOF. Though this is a standard result, we include the argument for convenience. With $a_f(\chi_i) = \langle\chi_i|f\rangle$, one calculates

$$\begin{aligned}
M\Bigl(\Bigl|f - \sum_{i=1}^{n} a_f(\chi_i)\,\chi_i\Bigr|^2\Bigr) \,&=\, \Bigl\langle f - \sum_{i=1}^{n} a_f(\chi_i)\,\chi_i \,\Bigm|\, f - \sum_{i=1}^{n} a_f(\chi_i)\,\chi_i\Bigr\rangle \\
&=\, \langle f|f\rangle \,-\, \sum_{i=1}^{n} \Bigl(a_f(\chi_i)\,\langle f|\chi_i\rangle + \overline{a_f(\chi_i)}\,\langle\chi_i|f\rangle\Bigr) \\
&\quad\, + \sum_{i,j=1}^{n} \overline{a_f(\chi_i)}\,a_f(\chi_j)\,\langle\chi_i|\chi_j\rangle \\
&=\, M\bigl(|f|^2\bigr) \,-\, 2\sum_{i=1}^{n} \bigl|a_f(\chi_i)\bigr|^2 \,+\, \sum_{i=1}^{n} \bigl|a_f(\chi_i)\bigr|^2
\end{aligned}$$

$$= M\big(|f|^2\big) - \sum_{i=1}^{n} \big|a_f(\chi_i)\big|^2,$$

where we used $\langle \chi_i | \chi_j \rangle = \delta_{ij}$ in the penultimate step. □

Lemma 4.6.7 ([15, Lemma 15.2])**.** *Let $f \in \mathrm{WAP}(G)$ and $\chi \in \widehat{G}$. Then, $a_{f\star\widetilde{f}}(\chi) = \big|a_f(\chi)\big|^2$.*

Proof. Using Proposition 4.5.11, we calculate

$$\begin{aligned} a_{f\star\widetilde{f}}(\chi) &= M_s\big((f\star\widetilde{f})(s)\overline{\chi}(s)\big) = M_s\big(M_t(f(t)\overline{f}(t-s))\overline{\chi}(s)\big) \\ &= M_t\big(M_s(f(t)\overline{f}(t-s)\overline{\chi}(s))\big) = M_t\big(f(t)M_s(\overline{f}(t-s)\overline{\chi}(s))\big) \\ &= M_t\big(f(t)\overline{\chi}(t)M_s(\overline{f}(t-s)\overline{\chi}(s-t))\big) \\ &= M_t\big(f(t)\overline{\chi}(t)\overline{M_s(f(t-s)\overline{\chi(t-s)})}\big) = a_f(\chi)\,\overline{a_f(\chi)}. \end{aligned}$$

Note that, in the last step, we have used the invariance of the mean to get rid of the t-dependence, and the independence of the mean from the Følner sequence in its definition to change the sign of s. □

Lemma 4.6.8. *Let $f \in \mathrm{SAP}(G)$, $f \geqslant 0$ and $M(f) = 0$. Then, $f = 0$.*

Proof. Suppose by way of contradiction that $f \neq 0$; then $f(x) > 0$ for some x. Since the mean is translation invariant, we may assume that $f(0) > 0$. Next, by the uniform continuity of f, there exists a precompact open set U so that, for all $x - y \in U$, we have $|f(x) - f(y)| < f(0)/4$.

By almost periodicity and Proposition 4.3.2, the set

$$P := \big\{t \in G : |f(t) - f(0)| < \tfrac{1}{4} f(0)\big\}$$

is relatively dense. Let K be compact so that $P + K = G$ and choose a function $g \in C_{\mathsf{c}}(G)$ so that $g \geqslant 1_{K+\overline{U}}$. Any element $x \in G$ can be written as $x = y + k$ with $y \in P$ and $k \in K$. It is easy to see that $f(y - s) \geqslant \frac{f(0)}{2}$ for all $s \in U$. From

$$\begin{aligned} (f * g)(x) &= \int_G f(x-t)g(t)\,\mathrm{d}\theta_G(t) \geqslant \int_{K+\overline{U}} f(x-t)\,\mathrm{d}\theta_G(t) \\ &\geqslant \int_{k+\overline{U}} f(x-t)\,\mathrm{d}\theta_G(t) = \int_{k+\overline{U}} f(y+k-t)\,\mathrm{d}\theta_G(t) \\ &\overset{s=t-k}{=} \int_{\overline{U}} f(y-s)\,\mathrm{d}\theta_G(s) \geqslant \frac{f(0)}{2}\,\theta_G(U), \end{aligned}$$

we see that $f * g \geqslant \frac{f(0)}{2}\,\theta_G(U)\,1_G$. As a result of Proposition 4.5.10, we know that $M(f)\int_G g\,\mathrm{d}\theta_G = M(f*g)$, so we have

$$0 \,=\, M(f)\int_G g\,\mathrm{d}\theta_G \,=\, M(f*g) \,\geqslant\, M\Big(\frac{f(0)}{2}\,\theta_G(U)1_G\Big) \,=\, \frac{f(0)}{2}\,\theta_G(U) \,>\, 0,$$

a contradiction. □

We have just seen that the sesquilinear form $\langle g|f\rangle = M(f\overline{g})$ is an inner product on $\mathrm{SAP}(G)$. This suggests to consider the Hilbert space completion $\mathcal{H}$ of $\mathrm{SAP}(G)$ into which $\mathrm{SAP}(G)$ is evidently faithfully embedded. We denote the corresponding norm by $\|.\|_{\mathcal{H}}$. In particular, the character group $\widehat{G}$ is embedded into it. Furthermore, using Proposition 4.5.9(iv), we see that G acts via isometries on $\mathrm{SAP}(G)$ relative to the inner product, and so G acts via isometries on the Hilbert space $\mathcal{H}$. The next result shows that this is as nice as it could possibly be.

Proposition 4.6.9. *The action of G on $\mathcal{H}$ decomposes it into a direct sum of G-eigenspaces, one for each $\chi \in \widehat{G}$, and indeed $\widehat{G}$ is an orthonormal Hilbert basis for $\mathcal{H}$.*

Proof. From Lemma 4.6.4, $\widehat{G}$ is an orthonormal set in $(\mathrm{SAP}(G), \langle\cdot|\cdot\rangle)$ and hence also in $\mathcal{H}$. We know that the linear span of $\widehat{G}$ is dense in $\mathrm{SAP}(G)$ in the strong topology (see the equivalence of statements (i) and (iv) in Theorem 4.3.5 on page 187) and since $\|.\|_{\mathcal{H}} \leqslant \|.\|_\infty$ by Proposition 4.5.9 (v), the linear span of $\widehat{G}$ is dense in $\mathcal{H}$. The orthonormality of the characters has already been established. □

Corollary 4.6.10. *For any $f \in \mathrm{SAP}(G)$, one has $f = 0$ if and only if $\langle\chi|f\rangle = a_f(\chi) = 0$ holds for all $\chi \in \widehat{G}$.* □

Lemma 4.6.11. *Let $f \in \mathrm{SAP}(G)$ be a function with the property that its Fourier series $\sum_{\chi\in\widehat{G}} a_f(\chi)\chi$ is uniformly convergent on G. Then, f is the limit of this series.*

Proof. Note that Bessel's inequality shows that at most countably many $a_f(\chi)$ can be non-zero; thus the convergence of this series is simple sequence convergence.

Let g be the uniform limit of $\sum_{\chi\in\widehat{G}} a_f(\chi)\chi$. Since each particular function $a_f(\chi)\chi$ lies in $\mathrm{SAP}(G)$, and since $\mathrm{SAP}(G)$ is closed under addition and uniform convergence, $g \in \mathrm{SAP}(G)$. Then, $a_{f-g}(\chi) = 0$ for all $\chi \in \widehat{G}$, and $f-g \in \mathrm{SAP}(G)$. By Corollary 4.6.10, this implies $f-g = 0$, which completes the proof. □

Theorem 4.6.12 (Parseval's equation [15, Thm. 15.2])**.** *Let $f \in \mathrm{WAP}(G)$. Then, $a_f(\chi) \neq 0$ for at most countably many χ, and one has*

$$M\bigl(|f|^2\bigr) = \sum_{\chi \in \widehat{G}} \bigl|a_f(\chi)\bigr|^2 .$$

Proof. We have $f \star \widetilde{f} \in \mathrm{SAP}(G)$ by Theorem 4.6.3, and its Fourier–Bohr coefficients are $|a_f(\chi)|^2$ by Lemma 4.6.7. Since, by Bessel's inequality, the series $\sum_{\chi \in \widehat{G}} |a_f(\chi)|^2$ is absolutely convergent, the Fourier series of $f \star \widetilde{f}$ is uniformly convergent, and thus, by Lemma 4.6.11, one has

$$f \star \widetilde{f} = \sum_{\chi \in \widehat{G}} a_{f \star \widetilde{f}}(\chi)\, \chi = \sum_{\chi \in \widehat{G}} |a_f(\chi)|^2\, \chi$$

as functions. Evaluating at 0, we get

$$M\bigl(|f|^2\bigr) \,=\, \bigl(f \star \widetilde{f}\bigr)(0) = \sum_{\chi \in \widehat{G}} |a_f(\chi)|^2\, \chi(0) = \sum_{\chi \in \widehat{G}} |a_f(\chi)|^2 ,$$

which proves the claim. □

The following result is a consequence of Lemma 4.6.6 in conjunction with Theorem 4.6.12.

Corollary 4.6.13 (Mean convergence in $\mathrm{WAP}(G)$ [15, Cor. 15.2.1])**.** *Consider $f \in \mathrm{WAP}(G)$, and let $\{\chi_n\}$ be all the characters χ with $a_f(\chi) \neq 0$. Then,*

$$\lim_{N \to \infty} M\left(\Bigl| f - \sum_{i=1}^{N} a_f(\chi_n)\, \chi_n \Bigr|^2 \right) \,=\, 0,$$

if there are infinitely many characters χ_n, or

$$M\left(\Bigl| f - \sum_{i=1}^{N} a_f(\chi_n)\, \chi_n \Bigr|^2 \right) \,=\, 0,$$

if there are exactly N of them. □

Recall the Bohr mapping

$$(.)_{\mathrm{B}} \colon \mathrm{SAP}(G) \longrightarrow C(G_{\mathrm{B}})$$

of Theorem 4.3.5 and Corollary 4.3.6, which is a G-invariant homeomorphism of algebras. Like all compact Abelian groups, G_{B} carries a unique normalised invariant Haar measure $\theta_{G_{\mathrm{B}}}$. We now give an important interpretation of the mean on G in terms of integration on G_{B}.

Theorem 4.6.14. *Let $f, g \in \mathrm{SAP}(G)$ and let $\theta_{G_{\mathrm{B}}}$ be the normalised Haar measure on G_{B}. Then,*

(i) $M(f) = \int_{G_{\mathrm{B}}} f_{\mathrm{B}} \,\mathrm{d}\theta_{G_{\mathrm{B}}}$;

(ii) $(f \star g)_{\mathrm{B}} = f_{\mathrm{B}} * g_{\mathrm{B}}$.

PROOF. In view of the G-homeomorphism $(.)_{\mathrm{B}}$, the mean M restricted to $\mathrm{SAP}(G)$ corresponds to a measure on G_{B}, and since M is a G-invariant mapping, this measure is G-invariant, too. Due to the continuity of the action of G on the space of measures on G_{B} and to the denseness of G in G_{B}, this measure must be a Haar measure on G_{B}, that is, it is $c\,\theta_{G_{\mathrm{B}}}$ for some constant c.

The proof of claim (i) now follows from the observation that

$$c \,=\, c\int_{G_{\mathrm{B}}} 1 \,\mathrm{d}\theta_{G_{\mathrm{B}}} \,=\, \theta_{G_{\mathrm{B}}}(1) \,=\, M(1|_G) \,=\, 1.$$

Given $f, g \in \mathrm{SAP}(G)$, one obtains

$$\bigl(f \star g\bigr)(t) \,=\, M_s\bigl(f(t-s)g(s)\bigr) \,=\, \int_{G_{\mathrm{B}}} f_{\mathrm{B}}(t-s)\, g_{\mathrm{B}}(s)\,\mathrm{d}\theta_{G_{\mathrm{B}}}(s) \,=\, \bigl(f_{\mathrm{B}} * g_{\mathrm{B}}\bigr)(t),$$

proving (ii). □

4.7. WAP = SAP ⊕ WAP$_0$

Definition 4.7.1. A function $f \in \mathrm{WAP}(G)$ is called *null weakly almost periodic* if $M(|f|) = 0$. The set of all null weakly almost periodic functions (within $\mathrm{WAP}(G)$) is denoted by $\mathrm{WAP}_0(G)$.

Since M is a continuous function on $\mathrm{WAP}(G)$, $\mathrm{WAP}_0(G)$ is a closed subset both of $\mathrm{WAP}(G)$ and of $C_{\mathrm{u}}(G)$ in the strong topology. In this section, we establish the important decomposition of $\mathrm{WAP}(G)$ announced in the title of this section.

Remark 4.7.2. For $f \in \mathrm{WAP}(G)$,

$$M(|f|) \,\leqslant\, \sqrt{M(|f|^2)} \,\leqslant\, \sqrt{\|f\|_\infty M(|f|)}.$$

The first inequality follows from Proposition 4.5.9(vii) (with g replaced by the constant function 1_G) and the second from the definition of M. With the inner product from Eq. (4.6.2), one finds

$$f \in \mathrm{WAP}_0(G) \iff M(|f|) = 0 \iff M\bigl(|f|^2\bigr) = 0 \iff \langle f|f\rangle = 0. \tag{4.7.1}$$

Thus, $\mathrm{WAP}_0(G)$ is the set of null elements of $\mathrm{WAP}(G)$ under $\langle\cdot|\cdot\rangle$. In particular, $\mathrm{WAP}_0(G)$ is a *subspace* of $\mathrm{WAP}(G)$. ◊

We are now going to make use of the semigroup $\mathcal{G}^*$ of operators

$$\mathcal{G}^* \,=\, \Bigl\{\sum_i a_i T_{t_i} : t_i \in G,\, a_i \geqslant 0, \sum_i a_i = 1\Bigr\},$$

where all sums have *finitely* many terms only; compare page 197.

Lemma 4.7.3. *For $i \in \{1,2\}$, let $h_i \in C_{\mathsf{u}}(G)$, $c_i \in \mathbb{C}$, $\varepsilon_i > 0$, and $T_i \in \mathcal{G}^*$ with*

$$\|c_i - T_i h_i\|_\infty < \varepsilon_i.$$

Then, with $T := T_1 T_2$,

$$\|c_i - T h_i\|_\infty < \varepsilon_i.$$

(*Here, c_i is being treated as the constant function $c_i 1_G$ on G.*)

Proof. Viewing c_2 as a constant function in $C_{\mathsf{u}}(G)$, one has $T_1 c_2 = c_2$. Now, one checks that

$$\|c_2 - T_1 T_2 h_2\|_\infty = \|T_1 c_2 - T_1 T_2 h_2\|_\infty \leqslant \|T_1\| \, \|c_2 - T_2 h_2\|_\infty < \varepsilon_2.$$

The same type of calculation works for c_1. □

Proposition 4.7.4 ([17, Lemma 1])**.** *Let $f \in \mathrm{SAP}(G)$ be a function with $f \geqslant 0$, $f(-x) = f(x)$ and $M(f) = 1$, and let $g \in \mathrm{WAP}(G)$. Then, $f \star g \in \mathcal{C}_g$.*

Proof. Recall the operators S_n of Proposition 4.5.2. Let $h_t := g\, T_t f$ for all $t \in G$ and let $0 < \varepsilon < \frac{1}{2}$. Using Definitions 4.5.5 and 4.6.1, one finds

$$\begin{aligned}(f \star g)(t) &= M_s\big(f(t-s)g(s)\big) = M_s\big(f(s-t)g(s)\big)\\ &= \lim_n S_n(g\, T_t f) = \lim_n S_n(h_t).\end{aligned}$$

Since $f \in \mathrm{SAP}(G)$, we know that $\{T_t f\}_t$ is precompact in the strong topology, and thus so is the set $\{g\, T_t f\}_t = \{h_t\}_t$, or equivalently, it is totally bounded. Using the equicontinuity of the operators S_n on $C_{\mathsf{u}}(G)$, see Proposition 4.5.2, we get, by a simple 3ε-argument, that

$$(f \star g)(t) = \lim_n S_n(h_t), \quad \text{uniformly in } t.$$

Fix n so that

$$\|(f \star g)(t) - S_n(h_t)\|_\infty < \varepsilon \quad \text{for all } t. \tag{4.7.2}$$

Since the functions $\{h_t\}_t$ are equi-uniformly continuous, we know (see Remark 4.5.4) that there exists a $T_1^* \in \mathcal{G}^*$ so that, for all $t \in G$,

$$\|S_n(h_t) - T_1^* h_t\|_\infty < \varepsilon. \tag{4.7.3}$$

Combining Eqs. (4.7.2) and (4.7.3), we obtain

$$\|(f \star g)(t) - T_1^* h_t\|_\infty < 2\varepsilon \quad \text{for all } t. \tag{4.7.4}$$

Since $M(f) = 1$, Proposition 4.5.6 implies $1_G = M(f) 1_G \in \mathcal{C}_f(\mathcal{G}^*) = \overline{O_f(\mathcal{G}^*)}$, and hence there exists a $T_2^* \in \mathcal{G}^*$ so that

$$\|1 - T_2^* f\|_\infty < \varepsilon. \tag{4.7.5}$$

When t is fixed, both $f \star g$ and 1 are constant functions in Eqs. (4.7.4) and (4.7.5), thus we can use Lemma 4.7.3 to replace both T_1^* and T_2^* by

their product, and hence assume from the outset that $T_1^* = T_2^* =: T^* = \sum_{i=1}^m a_i T_{t_i}$. We have

$$\begin{aligned}(T^* h_t)(s) &= \sum_{i=1}^m a_i \bigl(T_{t_i}(g T_t f)\bigr)(s) = \sum_{i=1}^m a_i \, (T_{t_i} g)(s) \, f(s-t-t_i) \\ &= \sum_{i=1}^m a_i \, f(s-t-t_i) \, (T_{t_i} g)(s), \quad \text{for all } s,t \in G.\end{aligned} \tag{4.7.6}$$

Also, from Eq. (4.7.5), with $b := \sum_{i=1}^m a_i f(-t_i)$,

$$|1-b| = \left|1 - \sum_{i=1}^m a_i f(-t_i)\right| = |1-(T^*f)(0)| < \varepsilon,$$

and thus, for $\varepsilon < \frac{1}{2}$, we have $\left|1-\frac{1}{b}\right| < 2\varepsilon$.

Substituting Eq. (4.7.6) into Eq. (4.7.4) and setting $s=t$, we get

$$\left|(f \star g)(t) - \sum_{i=1}^m a_i \, f(-t_i) \, (T_{t_i} \, g)(t)\right| \leqslant 2\varepsilon,$$

and hence

$$\begin{aligned}&\left|(f \star g)(t) - \sum_{i=1}^m \frac{a_i f(-t_i)}{b} \, (T_{t_i} \, g)(t)\right| \\ &\qquad \leqslant \left|(f \star g)(t) - \sum_{i=1}^m a_i \, f(-t_i) \, (T_{t_i} g)(t)\right| \\ &\qquad\quad + \left|\sum_{i=1}^m a_i \left(1-\frac{1}{b}\right) f(-t_i) \, (T_{t_i} g)(t)\right| \\ &\qquad \leqslant 2\varepsilon + 2\varepsilon \|f\|_\infty \|g\|_\infty .\end{aligned}$$

By the non-negativity of f and the definition of b, we obtain that

$$U := \sum_{i=1}^m \frac{a_i f(-t_i)}{b} T_{t_i} \in \mathcal{G}^*$$

and that

$$\|f \star g - U(g)\|_\infty < 2\varepsilon + 2\varepsilon \|f\|_\infty \|g\|_\infty .$$

Since we can find such a U for all $0 < \varepsilon < \frac{1}{2}$, we see that $f \star g \in \mathcal{C}_g$ (compare Eq. (4.4.5)), which is what we wanted to prove. □

Definition 4.7.5. A net $\{g_\alpha\}_{\alpha \in A} \subset C(G_{\mathrm{B}})$ on a directed set $(A, \geqslant)$ is an *approximate identity* (or *approximate unit*) if

(i) each g_α is a non-negative function satisfying $\int_{G_{\mathrm{B}}} g_\alpha \, \mathrm{d}\theta_{G_{\mathrm{B}}} = 1$;

(ii) the support of each g_α is a compact neighbourhood V_α of 0;

(iii) $V_\beta \subseteq V_\alpha$ if $\beta \geqslant \alpha$;

(iv) for each neighbourhood V of 0, there is an $\alpha \in A$ such that $V_\alpha \subseteq V$.

The conditions on the $\{V_\alpha\}_{\alpha\in A}$ imply that they form a basis for the neighbourhood filter of $\{0\}$.

Remark 4.7.6. We will have the opportunity to use approximate identities for $C_{\mathsf{u}}(G)$, too. The concept is the same: A net $\{g_\alpha\}_\alpha$ of $C_{\mathsf{u}}(G)$ satisfying conditions parallel to (i)–(iv) above. ♢

Lemma 4.7.7. *If $\{g_\alpha\}_{\alpha\in A}$ is an approximate identity for $C(G_{\mathrm{B}})$, then, for all $f \in C(G_{\mathrm{B}})$, we have*

$$\lim_\alpha f * g_\alpha \,=\, f$$

in the strong topology (sup-norm).

Proof. Choose $\varepsilon > 0$ and a neighbourhood V of 0 so that $|f(x) - f(y)| < \varepsilon$ if $x - y \in V$. By assumption, there is an α with $V_\beta \subseteq V$ for all $\beta \geqslant \alpha$. Then, for all $x \in G_{\mathrm{B}}$ and all $\beta \geqslant \alpha$,

$$\begin{aligned} \bigl|(f - f * g_\beta)(x)\bigr| \,&=\, \Bigl|f(x) - \int_{G_{\mathrm{B}}} f(y)\, g_\beta(x-y)\, \mathrm{d}\theta_{G_{\mathrm{B}}}(y)\Bigr| \\ &\leqslant \int_{G_{\mathrm{B}}} |f(x) - f(y)|\, g_\beta(x-y)\, \mathrm{d}\theta_{G_{\mathrm{B}}}(y) \,\leqslant\, \varepsilon, \end{aligned}$$

which completes the proof. □

Approximate identities always exist; compare [5, Def. 1.6].

Proposition 4.7.8. *Let $\{g_\alpha\}_{\alpha\in A} \subset C(G_{\mathrm{B}})$ be an approximate identity for $*$ and let $f_\alpha := g_\alpha\big|_G$. Then,*

(i) *$f_\alpha \in \mathrm{SAP}(G)$ and $f_\alpha \geqslant 0$;*

(ii) *$M(f_\alpha) = 1$;*

(iii) *$\lim_\alpha f \star f_\alpha = f$ for all $f \in \mathrm{SAP}(G)$ (in the strong topology);*

(iv) *$\|f_\alpha \star g\|_\infty \leqslant \|g\|_\infty$ for all $g \in \mathrm{WAP}(G)$;*

(v) *$T_t(f_\alpha \star g) = f_\alpha \star T_t g$ for all $t \in G$.*

Proof. Claim (i) is clear, while claim (ii) follows from Theorem 4.6.14. Let $f \in \mathrm{SAP}(G)$. Then, $f, f_\alpha, f\star f_\alpha \in \mathrm{SAP}(G)$ and, again by Theorem 4.6.14,

$$f \star f_\alpha \,=\, (f \star f_\alpha)_{\mathrm{B}}\big|_G \,=\, \bigl(f_{\mathrm{B}} * (f_\alpha)_{\mathrm{B}}\bigr)\big|_G \,=\, (f_{\mathrm{B}} * g_\alpha)|_G.$$

Since $\lim_\alpha f_{\mathrm{B}} * g_\alpha = f_{\mathrm{B}}$ in $C(G_{\mathrm{B}})$, one has $\lim_\alpha f \star f_\alpha = f_{\mathrm{B}}\big|_G = f$ in the strong topology on $C_{\mathsf{u}}(G)$. Finally, claims (iv) and (v) follow directly from the definition of the Eberlein convolution together with property (ii). □

Definition 4.7.9. A family of functions $\{f_\alpha\}_{\alpha\in A}$ of $\mathrm{SAP}(G)$ that arises from an approximate identity of G_{B} by the process of Proposition 4.7.8 is called an *approximate identity of* $\mathrm{SAP}(G)$.

Note. *For the remainder of this section,* $\{f_\alpha\}$ *will denote a fixed approximate identity for* $(\mathrm{SAP}(G),\star)$ *with the properties* $f_\alpha \geqslant 0$, $f_\alpha(-x) = f_\alpha(x)$ *and* $M(f_\alpha) = 1$.

For $f \in \mathrm{SAP}(G)$, we define an operator $N_f\colon \mathrm{WAP}(G) \longrightarrow \mathrm{WAP}(G)$ by

$$N_f(g) \,=\, g - f\star g.$$

We note that

$$H \,:=\, \{N_f : f \in \mathrm{SAP}(G)\} \tag{4.7.7}$$

is a convex Abelian semigroup that acts on $\mathrm{WAP}(G)$, with multiplication (that is, composition of operators)

$$N_f N_h \,=\, N_{f+h-f\star h};$$

see Remark 4.6.2. Let us abbreviate $N_\alpha := N_{f_\alpha}$.

Proposition 4.7.10 ([17, Lemma 2])**.** $\{N_\alpha\}$ *is a system of almost invariant integrals* (*relative to the sup-norm*) *for the action of* H *on* $\mathrm{WAP}(G)$.

Proof. We need to check the four conditions of Definition 4.4.33. Of these, condition (i) is clear and condition (ii) follows from the fact that $N_\alpha \in H$ (so in particular, $N_\alpha f \in \mathcal{C}_f(H)$ for all $f \in \mathrm{WAP}(G)$). For (iii), we see from Proposition 4.7.8(iv) that $\|N_\alpha\| \leqslant 2$, and then use Proposition 4.5.10.

To prove (iv), it suffices to observe that

$$\begin{aligned}\lim_\alpha \big(N_\alpha(g) - N_\alpha N_f(g)\big) \,&=\, \lim_\alpha \big(g - f_\alpha\star g - N_f(g) + f_\alpha\star N_f(g)\big)\\ &=\, \lim_\alpha \big(g - N_f(g) - f_\alpha\star(g - N_f(g))\big)\\ &=\, f\star g - \lim_\alpha (f_\alpha\star f\star g) \,=\, f\star g - f\star g \,=\, 0,\end{aligned}$$

where we have used $f\star g \in \mathrm{SAP}(G)$ and Proposition 4.7.8(iii). □

Theorem 4.7.11 ([17, Thm. 1])**.** *One has*

$$\mathrm{WAP}(G) \,=\, \mathrm{SAP}(G) \oplus \mathrm{WAP}_0(G);$$

that is, every $g \in \mathrm{WAP}(G)$ *possesses a unique decomposition* $g = g_{\mathsf{s}} + g_0$ *with* $g_{\mathsf{s}} \in \mathrm{SAP}(G)$ *and* $g_0 \in \mathrm{WAP}_0(G)$. *Moreover, if* g *is non-negative,* g_{s} *is also non-negative.*

Proof. Let $g \in \mathrm{WAP}(G)$. Since $\mathcal{C}_g(G)$ is weakly compact and $f_\alpha\star g \in \mathcal{C}_g(G)$ by Proposition 4.7.4, the net $\{f_\alpha\star g\}_\alpha$ has a weak cluster point, and thus the net $\{N_\alpha(g)\}$ has a weak cluster point g_0.

By Eberlein's ergodic theorem (Theorem 4.4.36), one gets

$$g_0 := \lim_\alpha N_\alpha(g) = \lim_\alpha (g - f_\alpha \star g) = g - \lim_\alpha (f_\alpha \star g),$$

and g_0 is H-invariant (with limits in the strong topology), with the semigroup H as defined in Eq. (4.7.7).

Let $g_{\mathsf{s}} := g - g_0$. Then, we have $g_{\mathsf{s}} = \lim_\alpha (f_\alpha \star g)$ in the sup-norm. Since $f_\alpha \star g \in \mathrm{SAP}(G)$ by Theorem 4.6.3 and since $\mathrm{SAP}(G)$ is closed in $C_{\mathsf{u}}(G)$, we see that $g_{\mathsf{s}} \in \mathrm{SAP}(G)$.

Now, for any $f \in \mathrm{SAP}(G)$, since $g_0 - f \star g_0 = N_f(g_0) = g_0$, we get $f \star g_0 = 0$. In particular, for $f = \chi \in \widehat{G}$, we obtain

$$0 = (\chi \star g_0)(t) = M_s(g_0(s)\chi(t-s)) = a_{g_0}(\chi)\,\chi(t),$$

so $a_{g_0}(\chi) = 0$ for all $\chi \in \widehat{G}$. Thus, by Parseval's equation (Theorem 4.6.12), $M\big(|g_0|^2\big) = 0$, and hence $g_0 \in \mathrm{WAP}_0(G)$ by Eq. (4.7.1).

Suppose that $g = h_{\mathsf{s}} + h_0$ is another decomposition of g into a strongly and a null weakly almost periodic function. Consequently, $|g_{\mathsf{s}} - h_{\mathsf{s}}| = |h_0 - g_0|$. The mean of the right-hand side is 0 by Eq. (4.7.1), and then the mean of the left-hand side is also 0. But $|g_{\mathsf{s}} - h_{\mathsf{s}}| \in \mathrm{SAP}(G)$ (see Corollary 4.3.6) and so, by Lemma 4.6.8, $g_{\mathsf{s}} - h_{\mathsf{s}} = 0$. This proves that the decomposition is unique.

The last claim of the theorem follows from $g_{\mathsf{s}} = \lim_\alpha (f_\alpha \star g)$ and from the fact that, for all α, one has $f_\alpha \geqslant 0$. □

Definition 4.7.12. We will refer to the formula $g = g_{\mathsf{s}} + g_0$ of Theorem 4.7.11 as the *Eberlein decomposition* of a weakly almost periodic function f.

Remark 4.7.13. Since the family of operators $\{N_\alpha\}$ is a system of almost invariant integrals, it follows that the projections

$$P_{\mathsf{s}}\colon\ \mathrm{WAP}(G) \longrightarrow \mathrm{SAP}(G)\colon \quad f \mapsto f_s$$
$$P_0\colon\ \mathrm{WAP}(G) \longrightarrow \mathrm{WAP}_0(G)\colon \quad f \mapsto f_0$$

arising from the decomposition of Theorem 4.7.11 are continuous linear mappings. Using Proposition 4.7.8(v), we see that they are also G-invariant mappings. ◊

Remark 4.7.14. Referring to the notation of Section 4.1.2, we note that, for all $f, g \in \mathrm{WAP}(G)$, $f^\dagger \star g^\dagger = (f \star g)^\dagger$ and then, since $f_\alpha = f_\alpha^\dagger$, also $N_\alpha(g^\dagger) = (N_\alpha(g))^\dagger$. From this, one has $(g_0)^\dagger = (g^\dagger)_0$ and $(g_{\mathsf{s}})^\dagger = (g^\dagger)_{\mathsf{s}}$, so we can write $g_0^\dagger$ and $g_{\mathsf{s}}^\dagger$ without ambiguity. ◊

4.8. Fourier transform of finite measures

Let us now expand on [AO1, Ch. 8] and describe the transition from almost periodic functions to almost periodic measures. The present section deals with *finite* regular Borel measures (that is, measures μ which do not

take infinite values ($\pm\infty$) on any subset of G); in the subsequent section, we deal with translation bounded (but not necessarily finite) measures.

Let G be an LCAG with dual group $\widehat{G}$. The *classical Fourier transform* is the mapping that sends $f \in L^1(G)$ to the function on $\widehat{G}$ defined by

$$\widehat{f}(\chi) \,=\, \int_G \overline{\chi}(x) f(x)\, \mathrm{d}x,$$

where the integration is relative to some fixed Haar measure on G.

We shall also use the *inverse Fourier transform* $\check{f}$ defined by $\check{f}(\chi) = \widehat{f}(\overline{\chi})$, or, equivalently, by $\check{\overline{f}} = \widehat{\overline{f}}$. We occasionally make use of this, proving things about the inverse Fourier transform by using the Fourier transform itself. These mappings can be defined similarly on $\widehat{G}$ and then, once the Haar measure on $\widehat{G}$ is suitably normalised, we have $\check{\widehat{f}} = f$ for all $f \in L^1(G)$ with $\widehat{f} \in L^1(\widehat{G})$, which explains the terminology of 'inverse' used here. For basic references, see [41] and [5].

We begin by recalling some familiar facts from the Fourier analysis of functions. For the convenience of the reader, we prove a couple of these.

Proposition 4.8.1. *Let G be an LCAG, let $t \in G$ and $f, g \in L^1(G)$. Then,*

(i) $\widehat{f+g} = \widehat{f} + \widehat{g}$;

(ii) $\widehat{f * g} = \widehat{f}\,\widehat{g}$ (*convolution theorem*);

(iii) $\widehat{f} \in C_0(\widehat{G})$ *and* $\|\widehat{f}\,\|_\infty \leqslant \|f\|_1$;

(iv) *If* $\widehat{f} \in L^1(\widehat{G})$, *one has* $\widehat{\widehat{f}} = f^\dagger$;

(v) $\widehat{T_t f}\,(\chi) = \overline{\chi(t)}\,\widehat{f}(\chi)$;

(vi) $\widehat{\widetilde{f}} = \widetilde{\widehat{f}}$.

Proof. Claims (i)–(iv) are standard [41]. For (v), one calculates

$$\begin{aligned}
\widehat{T_t f}(\chi) \,&=\, \int_G \overline{\chi(x)}\, T_t f(x)\, \mathrm{d}x \,=\, \int_G \overline{\chi(x)}\, f(-t+x)\, \mathrm{d}x \\
&= \int_G \overline{\chi(t)}\, \overline{\chi(-t+x)}\, f(-t+x)\, \mathrm{d}x \\
&= \overline{\chi(t)} \int_G \overline{\chi(-t+x)}\, f(-t+x)\, \mathrm{d}x \,=\, \overline{\chi(t)}\, \widehat{f}(\chi).
\end{aligned}$$

Similarly, recalling that $\widetilde{f}(\chi) = \overline{f(\chi^{-1})}$ in multiplicative notation, one has

$$\widehat{\overline{f}}(\chi) \,=\, \int_G \overline{\chi(x) f(x)}\, \mathrm{d}x \,=\, \overline{\int_G \chi(x) f(x)\, \mathrm{d}x} \,=\, \overline{\widehat{f}(\overline{\chi})} \,=\, \widetilde{\widehat{f}}(\chi),$$

where we used that $\overline{\chi} = \chi^{-1}$ in $\widehat{G}$, which proves claim (vi). □

Definition 4.8.2. Given a finite measure μ on an LCAG G, its *Fourier transform* is defined as the *function* on $\widehat{G}$ defined by

$$\chi \longmapsto \widehat{\mu}(\chi) := \int_G \overline{\chi(x)}\,\mathrm{d}\mu(x).$$

Since continuity on $\widehat{G}$ is defined by the compact-open topology, it is easy to see that $\widehat{\mu}$ is continuous.

Let us recall that, given a measure μ, we can define a positive measure $|\mu|$, called the *total variation measure* of μ, which satisfies

$$\int_G f(t)\,\mathrm{d}|\mu|(t) \;=\; \sup\left\{\left|\int_G g(t)\,\mathrm{d}\mu(t)\right| \,:\, g \in C_{\mathsf{c}}(G);\, |g| \leqslant f\right\} \tag{4.8.1}$$

for all non-negative functions $f \in C_{\mathsf{c}}(G)$. For details, we refer the reader to [35, Thm. 6.5.6] or [41, Def. 3.2.7]. Note that a measure μ on G is finite if and only if $|\mu|(G) < \infty$.

Lemma 4.8.3. *If μ is a finite measure on G, one has $\widehat{\mu} \in C_{\mathsf{u}}(\widehat{G})$. In addition, $\widehat{\mu}$ is bounded with $\|\widehat{\mu}\|_\infty \leqslant |\mu|(G)$.*

Proof. We first prove that $\widehat{\mu}$ is uniformly continuous. Let $\varepsilon > 0$. As μ is a finite regular Borel measure, $|\mu|(G)$ is finite and there exists some compact $K \subseteq G$ such that

$$|\mu|(K) \;>\; |\mu|(G) - \varepsilon.$$

The set

$$U \;=\; \left\{\chi \in \widehat{G} \,:\, |\chi(t) - 1| < \frac{\varepsilon}{|\mu|(K)+1} \text{ for all } t \in K\right\}$$

is open in $\widehat{G}$ and, for all $\phi, \chi \in \widehat{G}$ with $\phi - \chi \in U$, we have

$$\begin{aligned}
|\widehat{\mu}(\chi) - \widehat{\mu}(\phi)| \;&=\; \left|\int_G \left(\overline{\chi(t)} - \overline{\phi(t)}\right)\,\mathrm{d}\mu(t)\right| \\
&\leqslant \left|\int_K \left(\overline{\chi(t)} - \overline{\phi(t)}\right)\,\mathrm{d}\mu(t)\right| + \left|\int_{G\setminus K} \left(\overline{\chi(t)} - \overline{\phi(t)}\right)\,\mathrm{d}\mu(t)\right| \\
&\leqslant \int_K \left|\overline{\chi(t)} - \overline{\phi(t)}\right|\,\mathrm{d}|\mu|(t) \;+\; \int_{G\setminus K} \left|\overline{\chi(t)} - \overline{\phi(t)}\right|\,\mathrm{d}|\mu|(t) \\
&\leqslant \frac{\varepsilon\,|\mu|(K)}{|\mu|(K)+1} + 2|\mu|(G\setminus K) \;<\; 3\varepsilon.
\end{aligned}$$

Also, for all $\chi \in \widehat{G}$, we have

$$|\widehat{\mu}(\chi)| \;=\; \left|\int_G \overline{\chi(t)}\,\mathrm{d}\mu(t)\right| \;\leqslant\; |\mu|(G),$$

which shows that

$$\|\widehat{\mu}\|_\infty \;\leqslant\; |\mu|(G).$$

This proves that $\widehat{\mu} \in C_{\mathsf{u}}(\widehat{G})$, completing the proof. □

We recall the following key result from harmonic analysis.

Theorem 4.8.4 (Bochner's theorem [38, Thm. 4.4.19])**.** *A function ϕ on an LCAG G is positive definite and continuous if and only if there exists a finite positive measure ν on $\widehat{G}$ such that*

$$\phi(x) \,=\, \widehat{\nu}(x) \,=\, \int_{\widehat{G}} \overline{\chi(x)}\, \mathrm{d}\nu(\chi)$$

holds for all $x \in G$.

Proof. The hard part of the proof is to show the existence of the measure ν on $\widehat{G}$, for which we refer the reader to [41, Sec. 1.4.3]. The reverse implication is simple. The function ϕ is continuous by Lemma 4.8.3. To show the positive definiteness, let $t_1, \dots, t_n \in G$ and $a_1, \dots, a_n \in \mathbb{C}$. Then,

$$\begin{aligned}
\sum_{i,j=1}^{n} a_i\, \phi(t_i - t_j)\, \overline{a_j} \;&=\; \sum_{i,j=1}^{n} \int_{\widehat{G}} a_i\, \overline{\chi(t_i - t_j)}\, \overline{a_j}\, \mathrm{d}\nu(\chi) \\
&=\; \int_{\widehat{G}} \sum_{i,j=1}^{n} a_i\, \overline{\chi(t_i)}\, \chi(t_j)\, \overline{a_j}\, \mathrm{d}\nu(\chi) \\
&=\; \int_{\widehat{G}} \Big(\sum_{j=1}^{n} \overline{a_j}\, \chi(t_j) \Big) \Big(\sum_{i=1}^{n} a_i\, \overline{\chi(t_i)} \Big)\, \mathrm{d}\nu(\chi) \\
&=\; \int_{\widehat{G}} \Big| \sum_{j=1}^{n} \overline{a_i}\, \chi(t_j) \Big|^2\, \mathrm{d}\nu(\chi) \;\geqslant\; 0,
\end{aligned}$$

which completes the proof. □

Remark 4.8.5. If the measure ν from Theorem 4.8.4 is positive, $\mathcal{H} := L^2(\nu)$ is a Hilbert space with the inner product (in Dirac notation) given by

$$\langle f \,|\, g \rangle \,=\, \int_{\widehat{G}} \overline{f(\chi)}\, g(\chi)\, \mathrm{d}\nu(\chi),$$

and G acts continuously on $\mathcal{H}$ as a group of isometries via

$$(U_x f)(\chi) \,=\, x(\chi) f(\chi).$$

This provides an alternative to the proof offered in Theorem 4.8.4 since, by Section 4.3.4, the function

$$\phi(x) \,=\, \langle 1 \,|\, U_x 1 \rangle,$$

where 1 denotes the constant function with value 1, is positive definite. ◊

Lemma 4.8.6. *If μ is a finite measure on G, one has $\widehat{\mu} \in \mathrm{WAP}(\widehat{G})$.*

PROOF. Since μ is a finite measure, it can be written as a complex linear combination of (at most four) finite positive measures, which is also known as the complex Hahn–Jordan decomposition. Hence, by Theorem 4.8.4 (Bochner), $\widehat{\mu}$ is a complex linear combination of continuous positive definite functions, and thus is a weakly almost periodic function on $\widehat{G}$ by Proposition 4.3.8. □

Lemma 4.8.7 ([16]). *Let μ be a finite measure on G. Then, after identifying elements of G with their images in $\widehat{\widehat{G}}$ (so that we can think of them as functions on $\widehat{G}$), we have*

$$a_{\widehat{\mu}}(-x) \,=\, M((x)\widehat{\mu}) \,=\, \mu(\{x\}),$$

for all $x \in G$, where $M = M_{\widehat{G}}$ is the mean for the group $\widehat{G}$. In particular,

$$a_{\widehat{\mu}}(0) \,=\, M(\widehat{\mu}) \,=\, \mu(\{0\}),$$

where we refer to Definition 4.6.5 *for the notation.*

PROOF. The function $(x)\widehat{\mu}$ acts on $\widehat{G}$ by

$$\chi \,\longmapsto\, \chi(x)\widehat{\mu}(\chi) \,=\, \chi(x)\int_G \overline{\chi}(y)\,\mathrm{d}\mu(y).$$

Let $\{B_n\}$ be a Følner sequence in $\widehat{G}$. Then,

$$M((x)\widehat{\mu}) \,=\, \lim_n \frac{1}{\theta_{\widehat{G}}(B_n)} \int_{B_n} \chi(x) \int_G \overline{\chi}(y)\,\mathrm{d}\mu(y)\,\mathrm{d}\theta_{\widehat{G}}(\chi).$$

Since

$$\begin{aligned}\int_{B_n} |\chi(x)| \int_G |\overline{\chi}(y)|\;\mathrm{d}|\mu|(y)\,\mathrm{d}\theta_{\widehat{G}}(\chi) \,&=\, \int_{B_n}\int_G \mathrm{d}|\mu|(y)\,\mathrm{d}\theta_{\widehat{G}}(\chi)\\ &=\, \theta_{\widehat{G}}(B_n)\,|\mu|(G) \,<\, \infty,\end{aligned}$$

we can use dominated convergence and Fubini's theorem to interchange the order of limits and integrations to get

$$\begin{aligned}a_{\widehat{\mu}}(-x) \,=\, M_{\widehat{G}}((x)\widehat{\mu}) \,&=\, \int_G \lim_n \frac{1}{\theta_{\widehat{G}}(B_n)} \int_{B_n} \chi(x)\,\overline{\chi}(y)\;\mathrm{d}\theta_{\widehat{G}}(\chi)\,\mathrm{d}\mu(y)\\ &=\, \int_G M_{\widehat{G}}(x-y)\,\mathrm{d}\mu(y) \,=\, \mu(\{x\}).\end{aligned}$$

In the last step, we have used Lemma 4.6.4. □

We can now formulate the important analogue of Parseval's equation in our present setting.

Theorem 4.8.8 ([16, Thm. 1]). *Let μ be a finite measure. Then,*

$$\sum_{x\in G} \bigl|\mu(\{x\})\bigr|^2 \,=\, M\bigl(|\widehat{\mu}|^2\bigr),$$

where the sum on the left-hand side is effectively at most countable.

PROOF. By Lemma 4.8.7 together with Parseval's equation (Theorem 4.6.12), we get

$$\sum_{x\in G} \bigl|\mu(\{x\})\bigr|^2 \,=\, \sum_{x\in G} \bigl|a_{\widehat{\mu}}(\{x\})\bigr|^2 \,=\, M\bigl(|\widehat{\mu}|^2\bigr)$$

as claimed. □

The following result is now a consequence of this theorem in conjunction with Eq. (4.7.1) in Remark 4.7.2.

Corollary 4.8.9. *A finite measure μ is a continuous measure (no pure point part) if and only if $\widehat{\mu} \in \mathrm{WAP}_0(\widehat{G})$.* □

Note that this result can be interpreted as a generalisation of Wiener's criterion to the setting of general LCAGs; compare [AO1, Thm. 8.6].

Lemma 4.8.10. *Let μ be a finite pure point measure. Then, $\widehat{\mu} \in \mathrm{SAP}(\widehat{G})$.*

PROOF. Observe that

$$\mu \,=\, \sum_{x\in G} \mu(\{x\})\, \delta_x \quad \text{and} \quad \sum_{x\in G} \bigl|\mu(\{x\})\bigr| \,=\, |\mu|(G) \,<\, \infty, \tag{4.8.2}$$

where each sum is effectively finite or countable by standard arguments. Since μ is a pure point measure, one gets

$$\widehat{\mu}(\chi) \,=\, \int_G \overline{\chi(x)}\, \mathrm{d}\mu(x) \,=\, \sum_{x\in G} \overline{\chi(x)}\, \mu(\{x\}).$$

Identifying G and $\widehat{\widehat{G}}$, $\widehat{\mu}$ is the function on $\widehat{G}$ given by $\chi \mapsto \sum_{x\in G} \overline{\chi(x)}\mu(\{x\})$. From Eq. (4.8.2), we see that this function is uniformly convergent, and since it is the limit of a sequence of trigonometric polynomials, Theorem 4.3.5 shows that it lies in $\mathrm{SAP}(\widehat{G})$. □

Recall the notation of Remark 4.7.13, which we apply here to elements $\widehat{\mu}$ of $\mathrm{WAP}(\widehat{G})$. The Eberlein and the Lebesgue decomposition are related as follows.

Theorem 4.8.11. *Let μ be a finite measure, and let μ_{pp} and μ_{c} be its pure point part and its continuous part, respectively. Then,*

$$\widehat{\mu_{\mathsf{pp}}} \,=\, (\widehat{\mu})_{\mathsf{s}} \quad \textit{and} \quad \widehat{\mu_{\mathsf{c}}} \,=\, (\widehat{\mu})_0.$$

Thus, $\widehat{\mu}$ is decomposed as

$$\widehat{\mu} \,=\, \widehat{\mu_{\mathsf{pp}}} + \widehat{\mu_{\mathsf{c}}}$$

into its strongly and null weakly almost periodic parts.

PROOF. Since μ is finite, μ_{pp} and μ_{c} are finite pure point, respectively continuous, measures. By Lemma 4.8.6, their Fourier transforms are weakly almost periodic on $\widehat{G}$. By Lemma 4.8.10 and Corollary 4.8.9, their Fourier transforms are $\widehat{\mu_{\mathsf{pp}}} \in \mathrm{SAP}(\widehat{G})$ and $\widehat{\mu_{\mathsf{c}}} \in \mathrm{WAP}_0(\widehat{G})$. Thus, $\widehat{\mu} = \widehat{\mu_{\mathsf{pp}}} + \widehat{\mu_{\mathsf{c}}}$ is a decomposition of the weakly almost periodic function $\widehat{\mu}$ into strongly and null weakly almost periodic components. As such a decomposition is unique by Theorem 4.7.11, it is the desired decomposition. □

4.9. Fourier transformable measures

If μ is a measure on G and f is a measurable function that satisfies $|f| \in L^1(|\mu|)$, we denote the pairing of μ and f by

$$\langle \mu, f \rangle_G := \int_G f(x)\, \mathrm{d}\mu(x). \tag{4.9.1}$$

Whenever the meaning is clear, we will omit the index G and simply write $\langle \mu, f \rangle$. In the spirit of [1], the pairing $\langle \mu, f \rangle$ is always understood to include the integrability condition $|f| \in L^1(|\mu|)$.

Now, if μ is a finite measure on G, then $\widehat{\mu}$ is a function, and hence also a measure, on $\widehat{G}$. For any $g \in C_{\mathsf{c}}(\widehat{G})$, one finds that

$$\langle \widehat{\mu}, g \rangle_{\widehat{G}} = \langle \mu, \widehat{g} \rangle_G, \tag{4.9.2}$$

by directly using the definitions, identifying $\widehat{\widehat{G}}$ with G, and interchanging the order of integration. The basic idea for forming the Fourier transform of an unbounded measure μ on G is that it should be the measure on $\widehat{G}$ that satisfies the same identity as in Eq. (4.9.2).

The primary difficulty faced here is that the space $C_{\mathsf{c}}(\widehat{G})$ of test functions for measures on $\widehat{G}$ is not carried into $C_{\mathsf{c}}(G)$ in the dual group (rather it is carried into, but not onto, the space of square integrable $C_0(G)$ functions) and there arises the question of whether the right-hand side makes sense.[9] In fact, it does not make sense in general, even for translation bounded measures. However, there is a way in which to define the Fourier transform of certain translation bounded measures. In this section, we review one common concept of Fourier transformable measures and deduce some of their properties. Later, in Section 4.11, we shall see that the translation bounded measures of greatest importance to us, namely the translation bounded positive definite measures, are transformable. These measures are also weakly almost periodic and we can obtain precisely the type of result that we would expect from our theory of almost periodic functions.

As we use them, all measures are assumed to be Radon measures.

[9] $C_0(G)$ is the space of all continuous functions f which 'vanish at infinity' in the sense that, for all $\varepsilon > 0$, there exists a compact subset K of G so that $|f(x)| < \varepsilon$ for all $x \in G \backslash K$.

Definition 4.9.1. A positive measure μ on G is a *Radon measure* if it is locally finite and if, for all Borel sets $B \subseteq G$, one has

$$\mu(B) \,=\, \sup\{\mu(K) : K \subseteq B,\ K \text{ compact}\}.$$

More generally, a measure on G is a Radon measure if its four components (the positive and negative parts of its real and imaginary parts) are positive Radon measures.

Remark 4.9.2. For finite measures, this concept corresponds to regular Borel measures. In classical measure theory, it is often assumed that, for a real signed measure, at most one of the negative or positive components can be infinite. With this convention, a linear combination of measures might not be a measure, which would create issues for us. Because of this, in Definition 4.9.1, we follow the approach of Bourbaki [7, 8, 9] and Weil [50]; see also [12, 38, 45]. It is important to emphasise here that, with this approach, only precompact Borel sets are guaranteed to be measurable. In particular, compact sets are measurable.

For example, the measure $\delta_{2\mathbb{Z}} - \delta_{2\mathbb{Z}+1}$ is a difference between two positive Radon measures, thus it is a Radon measure on $\mathbb{R}$. However, we cannot assign a finite or infinite value to $\big(\delta_{2\mathbb{Z}} - \delta_{2\mathbb{Z}+1}\big)\,(\mathbb{R})$. $\Diamond$

The Riesz representation theorem allows us to identify the Radon measures with the functionals on $C_{\mathsf{c}}(G)$ that are continuous in the sense of Eq. (4.9.3) below.

Theorem 4.9.3 (Riesz representation theorem [12])**.** *Let $L\colon C_{\mathsf{c}}(G) \longrightarrow \mathbb{C}$ be a linear functional. Then, the following statements are equivalent.*

(i) *There exists a Radon measure μ on G such that, for all $f \in C_{\mathsf{c}}(G)$, we have*

$$L(f) \,=\, \int_G f(t)\,\mathrm{d}\mu(t).$$

(ii) *For each compact set $K \subseteq G$, there exists a constant c_K such that*

$$|L(f)| \,\leqslant\, c_K \|f\|_\infty \tag{4.9.3}$$

holds for all $f \in C_{\mathsf{c}}(G)$ with $\mathrm{supp}(f) \subseteq K$. $\square$

Remark 4.9.4. Let us add some comments.

(i) Any positive linear functional $L\colon C_{\mathsf{c}}(G) \longrightarrow \mathbb{C}$ satisfies Eq. (4.9.3), which means that it is a positive Radon measure.

(ii) Given a measure μ, the corresponding total variation measure $|\mu|$, compare Eq. (4.8.1), can be defined on $f \in C_{\mathsf{c}}(G)$ with $f \geqslant 0$ via

$$|\mu|(f) \,=\, \sup\big\{|\mu(g)| : g \in C_{\mathsf{c}}(G),\, |g| \leqslant f\big\},$$

which can be extended to a positive measure by linearity.

In general, given a linear functional $L\colon C_{\mathsf{c}}(G) \longrightarrow \mathbb{C}$, it is easy to show that the mapping defined by

$$0 \leqslant f \longmapsto \sup\bigl\{|L(g)| : g \in C_{\mathsf{c}}(G),\, |g| \leqslant f\bigr\}$$

on non-negative functions is finite and can be extended to a positive functional $|L|\colon C_{\mathsf{c}}(G) \longrightarrow \mathbb{C}$ if and only if L satisfies Eq. (4.9.3); see [40, App. C] for details. ◊

The theory begins with a special class of test functions.

Definition 4.9.5. We define

$$\mathcal{K}_2(G) := \operatorname{span}_{\mathbb{C}}\bigl\{f * g : f, g \in C_{\mathsf{c}}(G)\bigr\};$$
$$\widehat{\mathcal{K}_2}(G) := \bigl\{\widehat{f} : f \in \mathcal{K}_2(G)\bigr\} = \bigl\{\check{f} : f \in \mathcal{K}_2(G)\bigr\}.$$

Lemma 4.9.6. *Let G be an LCAG. Then, the space $\mathcal{K}_2(G)$ has the following properties.*

(i) *$\mathcal{K}_2(G) \subseteq C_{\mathsf{c}}(G)$, and $\mathcal{K}_2(G)$ is closed under the convolution product;*

(ii) *$\widehat{\mathcal{K}_2}(G)$ is closed under multiplication;*

(iii) *$\mathcal{K}_2(G)$ is dense in $C_{\mathsf{c}}(G)$ in the strong topology;*

(iv) *$\mathcal{K}_2(G)$ is closed under multiplication by characters;*

(v) *$\widehat{\mathcal{K}_2}(G) \subseteq L^1(\widehat{G})$.*

Sketch of proof. Property (i) is clear, and (ii) follows because convolution and multiplication are interchanged by the Fourier transform (convolution theorem). For (iii), use an approximate identity $\{f_\alpha\}$ for the convolution on G; see Remark 4.7.6 and Lemma 4.7.7.

For claim (iv), let $\chi \in \widehat{G}$ and $f_1, f_2 \in C_{\mathsf{c}}(G)$. Then,

$$\begin{aligned}\bigl(\chi(f_1 * f_2)\bigr)(x) &= \chi(x) \int_G f_1(x-t)\, f_2(t)\, \mathrm{d}t \\ &= \int_G \chi(x-t)\, f_1(x-t)\chi(t)\, f_2(t)\, \mathrm{d}t = \bigl((\chi f_1) * (\chi f_2)\bigr)(x),\end{aligned}$$

which shows that $\chi(f_1 * f_2) \in \mathcal{K}_2(G)$; conclude by taking linear combinations. Finally, for claim (v), see [41, Thm. 1.5]. □

Definition 4.9.7. A measure μ on G is called *Fourier transformable*, or transformable for short, if there exists a measure $\widehat{\mu}$ on $\widehat{G}$, called the *Fourier transform* of μ, so that, for all $f \in C_{\mathsf{c}}(G)$,

$$\check{f} \in L^2(\widehat{\mu}) \quad \text{and} \quad \bigl\langle \mu, f * \widetilde{f} \bigr\rangle = \bigl\langle \widehat{\mu}, (f * \widetilde{f})^{\vee} \bigr\rangle = \bigl\langle \widehat{\mu}, |\check{f}\,|^2 \bigr\rangle, \tag{4.9.4}$$

where $\check{f} \in L^2(\widehat{\mu})$ means $|\check{f}\,| \in L^2(|\widehat{\mu}|)$. Note further that requiring $\check{f} \in L^2(\widehat{\mu})$ for all $f \in C_{\mathsf{c}}(G)$ is equivalent to requiring $\widehat{f} \in L^2(\widehat{\mu})$ for all $f \in C_{\mathsf{c}}(G)$.

Remark 4.9.8. Let us note that the requirement $\widehat{f} \in L^2(\widehat{\mu})$ for all $f \in C_{\mathsf{c}}(G)$ might be too restrictive in some situations. In particular, if $G = \mathbb{R}^d$, some recent work [29, 48, 31, 4] suggests that a wider concept of transformability is possible by a skilful use of tempered distributions.

In fact, it is shown in [47, Thm. 4.3] that a measure μ on $\mathbb{R}^d$ is Fourier transformable as a measure in our above sense when μ is tempered as a distribution and when the Fourier transform $\widehat{\mu}$ in the distribution sense is a translation bounded measure [47, Thm. 5.2]. This gives a clear indication where an extension is possible. ♢

Using the complex polarisation identity

$$\begin{aligned} f * \widetilde{g} \,=\, \frac{1}{4}\Big(& \big[(f+g) * \widetilde{(f+g)} - (f-g) * \widetilde{(f-g)}\big] \\ & + \mathrm{i}\big[(f+\mathrm{i}g) * \widetilde{(f+\mathrm{i}g)} - (f-\mathrm{i}g) * \widetilde{(f-\mathrm{i}g)}\big]\Big), \end{aligned}$$

we obtain the following useful equivalent definitions of the Fourier transform of a measure; see [AO1, Ch. 8] for various examples.

Proposition 4.9.9. *Let μ and $\widehat{\mu}$ be measures on G and $\widehat{G}$, respectively. Then, the following statements are equivalent.*

(i) *The measure μ is transformable with Fourier transform $\widehat{\mu}$;*
(ii) *For all $g \in \mathcal{K}_2(G)$, one has $\breve{g} \in L^1(\widehat{\mu})$ and $\langle \mu, g\rangle = \langle \widehat{\mu}, \breve{g}\rangle$;*
(iii) *For all $f \in \widehat{\mathcal{K}}_2(G)$, one has $f \in L^1(\widehat{\mu})$ and $\langle \mu, \widehat{f}\,\rangle = \langle \widehat{\mu}, f\rangle$.* □

Regarding (ii), to see that $g \in \mathcal{K}_2(G)$ implies that $\widehat{g} \in L^1(\widehat{\mu})$, it is enough to verify this for $g = f * \widetilde{f}$ with $f \in C_{\mathsf{c}}(G)$, see Eq. (4.9.4). Then, the square integrability of f implies that of $\widehat{f}$, and so $\widehat{g}$ is integrable.

At this point, we gather properties of transformable measures and their transforms. The important existence result is Theorem 4.11.5.

Proposition 4.9.10. *The space $\widehat{\mathcal{K}_2}(G)$ is dense in $C_0(\widehat{G})$ in the sup-norm topology.* □

This is a simple consequence of Lemma 4.9.6(iii) and the following result.

Lemma 4.9.11. *The set $\{\widehat{f} : f \in C_{\mathsf{c}}(G)\}$ is dense in $C_0(\widehat{G})$.*

Proof. Let $h \in C_0(\widehat{G})$ and $\varepsilon > 0$. Then, there exists $g \in C_{\mathsf{c}}(\widehat{G})$ so that $\|h - g\|_\infty < \varepsilon$. By the Riemann–Lebesgue lemma [41, 38], $\breve{g} \in C_0(G)$. Then, there exists $f \in C_{\mathsf{c}}(G)$ so that $\|f - \breve{g}\|_1 < \varepsilon$. Consequently, $\|\widehat{f} - g\|_\infty < \varepsilon$, which implies $\|\widehat{f} - h\|_\infty < 2\varepsilon$. □

Corollary 4.9.12. *For each compact set $K \subseteq \widehat{G}$, there exists a continuous function $f \in C_{\mathsf{c}}(G)$ with $\widehat{f} \geqslant 1_K$.* □

PROOF. Let $K \subseteq \widehat{G}$ be compact. There certainly exists a function $g \in C_0(\widehat{G})$ with $g > 1_K$. Let $m := \min_{x\in K} |g(x)-1| > 0$. Then, by Lemma 4.9.11, there is a function $h \in C_{\mathsf{c}}(G)$ with $\|g-\widehat{h}\|_\infty < m$. Consequently, we have $\widehat{h}(x) \geqslant 1$ for all $x \in K$.

Let $f = h * \widetilde{h}$. Then, $f \in C_{\mathsf{c}}(G)$ and $\widehat{f} = \bigl|\widehat{h}\bigr|^2 \geqslant 1_K$. □

For an alternative (and simple) proof of Corollary 4.9.12, we refer the reader to [5, Prop. 2.4].

Theorem 4.9.13 ([1, Thm. 2.1])**.** *If the measure μ is Fourier transformable, μ and $\widehat{\mu}$ determine each other uniquely via Eq.* (4.9.4)*.*

PROOF. Let μ_1, μ_2 be transformable measures on G with $\widehat{\mu_1} = \widehat{\mu_2}$. Then, for all $g \in \mathcal{K}_2(G)$, we have

$$\langle \mu_1, g\rangle \,=\, \langle \widehat{\mu_1}, \check{g}\rangle \,=\, \langle \widehat{\mu_2}, \check{g}\rangle \,=\, \langle \mu_2, g\rangle$$

and $\mu_1 = \mu_2$ by the denseness of $\mathcal{K}_2(G)$ in $C_{\mathsf{c}}(G)$.

Let us now suppose that, for a measure μ, there exist two measures $(\widehat{\mu})_1$ and $(\widehat{\mu})_2$ for which Eq. (4.9.4) holds. Let $f, g \in K_2(G)$. Then, by Eq. (4.9.4), we have

$$\bigl\langle \check{g}, \check{f}(\widehat{\mu})_1\bigr\rangle \,=\, \bigl\langle \check{g}\check{f}, (\widehat{\mu})_1\bigr\rangle \,=\, \bigl\langle f*g, \mu\bigr\rangle \,=\, \bigl\langle \check{g}\check{f}, (\widehat{\mu})_2\bigr\rangle \,=\, \bigl\langle \check{g}, \check{f}(\widehat{\mu})_2\bigr\rangle.$$

Now, by the definition of Fourier transformability, the measures $\check{f}(\widehat{\mu})_1$ and $\check{f}(\widehat{\mu})_2$ are finite for any fixed $f \in \mathcal{K}_2(G)$. Therefore, by the Riesz representation theorem, see Thereom 4.9.3 above, they are continuous linear functionals on $C_0(\widehat{G})$. Since these functionals agree on $\widehat{\mathcal{K}_2}(G)$, which is dense in $C_0(\widehat{G})$, they are equal as finite measures on $\widehat{G}$.

Therefore, for all $f \in \mathcal{K}_2(G)$, we have $\check{f}(\widehat{\mu})_1 = \check{f}(\widehat{\mu})_2$. The claim now follows from Corollary 4.9.12. □

Lemma 4.9.14 ([1, Thm. 2.2])**.** *Finite measures as well as L^1-functions are Fourier transformable, and their Fourier transforms as measures coincide with their classical Fourier transforms.*

PROOF. Let μ be a finite measure and $g \in \mathcal{K}_2(G)$. Then, $\check{g} \in L^1(\widehat{G})$ by Lemma 4.9.6. Let f be the classical Fourier transform of μ. Then, we have $\check{g}f \in L^1(\widehat{G})$, which shows that $\check{g} \in L^1(f)$.

Moreover, $\mu * g^\dagger \in L^1(G)$ is continuous and $\widehat{\mu * g^\dagger} = f\check{g}$. By taking the inverse Fourier transform and evaluating at 0, we get

$$\langle \mu, g\rangle \,=\, (\mu * g^\dagger)(0) \,=\, \int_{\widehat{G}} f\,\check{g}\,\mathrm{d}\theta_{\widehat{G}} \,=\, \langle f\theta_{\widehat{G}}, \check{g}\rangle,$$

which shows that μ is Fourier transformable, and $\widehat{\mu} = f\theta_{\widehat{G}}$. For L^1-functions, it is now enough to observe that the classical Fourier theory is compatible with the embedding of $L^1(G)$ into the space of all finite measures on G. □

We next prove that the Fourier transform of a finite measure is also Fourier transformable. Recall that a function ϕ on G can always be considered as a measure on G via $\phi\,\theta_G$.

Lemma 4.9.15. *Let ν be a finite measure on $\widehat{G}$ and let $\phi = \widehat{\nu}$ be its Fourier transform. Then, ϕ is transformable as a measure, and its Fourier transform is $\nu^{\dagger}$.*

Proof. Let $f \in C_{\mathsf{c}}(G)$. Since ν is a finite measure, $\widehat{f} \in L^2(\nu)$. Now, $|\widehat{f}\,|^2\nu$ is a finite measure as well. For each $x \in G$, we then have

$$\begin{aligned}\int_{\widehat{G}} \chi(x)\,\big|\widehat{f}\,\big|^2(\chi)\,\mathrm{d}\nu^{\dagger}(\chi) &= \int_{\widehat{G}} \chi(x) \int_G \overline{\chi}(y)\big(f * \widetilde{f}\,\big)(y)\,\mathrm{d}y\,\mathrm{d}\nu^{\dagger}(\chi)\\ &= \int_G \int_{\widehat{G}} \chi(x)\overline{\chi}(y)\big(f * \widetilde{f}\,\big)(y)\,\mathrm{d}\nu(-\chi)\,\mathrm{d}y\\ &= \int_G \big(f * \widetilde{f}\,\big)(y) \int_{\widehat{G}} \overline{\chi(x-y)}\,\mathrm{d}\nu(\chi)\,\mathrm{d}y\\ &= \int_G \big(f * \widetilde{f}\,\big)(y)\,\phi(x-y)\,\mathrm{d}y \;=\; \big(\phi * f * \widetilde{f}\,\big)(x).\end{aligned}$$

Evaluating at 0, we get

$$\big\langle \phi\theta_G, f^{\dagger} * \widetilde{f^{\dagger}}\big\rangle \;=\; \big\langle \nu^{\dagger}, \big|\widehat{f}\,\big|^2\big\rangle \;=\; \big\langle \nu^{\dagger}, \big|\widetilde{f^{\dagger}}\,\big|^2\big\rangle,$$

from which we obtain the desired transformability using Definition 4.9.7 (with $f^{\dagger}$ replacing f). □

Remark 4.9.16. The point of this lemma is that ϕ need not be Fourier transformable as a function, since there is no assumption on its support or integrability. ♢

Definition 4.9.17. A measure μ is called *translation* (or *shift*) *bounded* if, for every compact set K in G, there exists a constant $c_K \geqslant 0$ so that

$$\|\mu\|_K \;:=\; \sup_{x\in G} |\mu|(x+K) \;\leqslant\; c_K\,.$$

We will denote the space of translation bounded measures by $\mathcal{M}^{\infty}(G)$.

Definition 4.9.18. Two measures μ and ν on G are called *convolvable* if, for all $f \in C_{\mathsf{c}}(G)$, the function $(x,y) \mapsto f(x+y)$ is in $L^1\big(|\mu| \times |\nu|\big)$. In this case, the *convolution* of μ and ν is the measure $\mu * \nu$ defined by

$$\langle \mu * \nu, f\rangle \;=\; \int_G \int_G f(x+y)\,\mathrm{d}\mu(x)\,\mathrm{d}\nu(y).$$

Lemma 4.9.19 ([1, Thm. 1.2])**.** *If μ and ν are measures on G with μ translation bounded and ν finite, then μ and ν are convolvable.*

PROOF. For any function $f \in C_{\mathsf{c}}(G)$, we claim that $|f| * |\mu^\dagger|$ is a bounded function in $C_{\mathsf{u}}(G)$.

Let $-K$ be the support of f. Choose any compact neighbourhood R of 0 in G and find a uniform bound C for $|\mu^\dagger|(x + R + K)$ with $x \in G$. Choose $\varepsilon > 0$ and find a neighbourhood $U \subset R$ of 0 in G so that $u - v \in U$ implies that $\bigl||f|(u) - |f|(v)\bigr| < \varepsilon$. Now, for all x, y with $x - y \in U$ and for all z, one has $\bigl||f|(x - z) - |f|(y - z)\bigr| < \varepsilon$, so this term certainly vanishes unless $z \in x + K$ or $z \in y + K$. In either case, $z \in x + R + K$. Computing

$$\int \bigl||f|(x - z) - |f|(y - z)\bigr| \,\mathrm{d}|\mu^\dagger|(z),$$

we now see that this expression is bounded by εC as long as $x - y \in U$, and this shows that $|f| * |\mu^\dagger|$ is uniformly continuous. The boundedness is also easy to see, so $|f| * |\mu^\dagger| \in C_{\mathsf{u}}(G)$.

Since $|\nu|$ is finite, it follows that $|f| * |\mu^\dagger| \in L^1(|\nu|)$. Therefore,

$$\int_{G \times G} |f(x + y)| \,\mathrm{d}|\mu|(x) \,\mathrm{d}|\nu|(y) = \int_G \bigl(|f| * |\mu^\dagger|\bigr)(y) \,\mathrm{d}|\nu|(y) < \infty,$$

and we are done. □

Corollary 4.9.20 ([1, Cor. 1.1])**.** *If μ is a translation bounded measure on G and $f \in L^1(G)$, then μ and f are convolvable as measures.* □

If $f \in C_{\mathsf{c}}(G)$, then $f\theta_G$ is the finite measure $h \mapsto \int_G hf \,\mathrm{d}\theta_G$. This evidently is an absolutely continuous measure on G with respect to θ_G. In particular, if μ is a translation bounded measure, we can use Lemma 4.9.19 to obtain the measure

$$\begin{aligned}(f\theta_G) * \mu \colon\ h \longmapsto \int_G \int_G h(x + y) \,\mathrm{d}(f\theta_G)(x) \,\mathrm{d}\mu(y) \\ = \int_G \int_G h(x + y) f(x) \,\mathrm{d}\theta_G(x) \,\mathrm{d}\mu(y) \\ = \int_G \int_G h(z) f(z - y) \,\mathrm{d}\mu(y) \,\mathrm{d}\theta_G(z),\end{aligned}$$

which is the absolutely continuous measure defined by the function

$$z \longmapsto \int_G f(z - y) \,\mathrm{d}\mu(y) \in C_{\mathsf{u}}(G). \tag{4.9.5}$$

Thus, the usual definition of $f * \mu$ as the continuous *function* of Eq. (4.9.5) is consistent with its definition via the convolution of two measures.

If μ is itself an absolutely continuous measure of the form $g\theta_G$, where $g \in C_{\mathsf{u}}(G)$, then this becomes the absolutely continuous measure with respect

to the function

$$z \longmapsto \int_G f(z-y)\, g(y)\, \mathrm{d}\theta_G(y) \,=\, (f * g)(z), \tag{4.9.6}$$

which shows that convolution of measures is consistent with convolution of continuous functions: Indeed, for $f \in C_{\mathsf{c}}(G)$ and $g \in C_{\mathsf{u}}(G)$, one has

$$f * (g\theta_G) \,=\, (f\theta_G) * (g\theta_G) \,=\, (f * g)\, \theta_G. \tag{4.9.7}$$

The following proposition provides an alternative characterisation of translation bounded measures that we shall use further.

Proposition 4.9.21 ([1, Thm. 1.1])**.** *For a measure μ, we have $\mu \in \mathcal{M}^\infty(G)$ if and only if, for all $f \in C_{\mathsf{c}}(G)$, the convolution satisfies $f * \mu \in C_{\mathsf{u}}(G)$.*

Proof. The proof of the 'only if' part is effectively the same as the one used in the proof of Lemma 4.9.19, via identifying a finite measure with its Radon–Nikodym density relative to θ_G.

Let us consider the converse direction. Assume that, for all $f \in C_{\mathsf{c}}(G)$, $\mu * f \in C_{\mathsf{u}}(G)$. Fix a compact subset K of G, define the Banach space $C(G,K) := \{f \in C_{\mathsf{c}}(G) : \mathrm{supp}(f) \subseteq K\}$, and consider the mapping

$$F\colon\, C(G,K) \longrightarrow C_{\mathsf{u}}(G) \quad \text{defined by } f \longmapsto \mu * f \text{ for all } f.$$

We prove that F is continuous by means of the closed graph theorem. To do so, we need to prove that, if a sequence $\{f_n\} \longrightarrow f$ in $C(G,K)$ and $\{\mu * f_n\} \longrightarrow g$ in $C_{\mathsf{u}}(G)$, then $g = \mu * f$. Indeed,

$$\begin{aligned} \big|\big(\mu * f_n - \mu * f\big)(x)\big| &\leqslant \int_{x-K} \big|f_n(x-t) - f(x-t)\big|\, \mathrm{d}|\mu|(t) \\ &\leqslant \|f_n - f\|_\infty\, |\mu|(x-K), \end{aligned}$$

from which we have pointwise convergence of $\{\mu * f_n\} \longrightarrow \mu * f$. But we also have $\{\mu * f_n\} \longrightarrow g$ in the sup-norm, so $\mu * f = g$.

Continuity of F implies the existence of a constant a_K with the estimate $\|\mu * f\|_\infty \leqslant a_K \|f\|_\infty$, valid for all $f \in C(G,K)$.

Let B be compact, with $B^\circ \supset K$, and let $x \in G$. Choose $f \in C_{\mathsf{c}}(G)$ so that $1_{x+K} \leqslant f \leqslant 1_{x+B^\circ}$, which is clearly possible. Then, by the definition of the total variation measure in Eq. (4.8.1), we have

$$\begin{aligned} |\mu|(x+K) \,\leqslant\, |\mu|(f) \,&=\, \sup\big\{|\mu(g)| : g \in C_{\mathsf{c}}(G),\, |g| \leqslant f\big\} \\ &\leqslant\, \sup\big\{|\mu(g)| : g \in C_{\mathsf{c}}(G),\, \mathrm{supp}(g) \subseteq x+B,\, \|g\|_\infty \leqslant 1\big\} \\ &=\, \sup\big\{|(\mu * f^\dagger)(x)| : f \in C_{\mathsf{c}}(G),\, \mathrm{supp}(f) \subseteq B,\, \|f\|_\infty \leqslant 1\big\} \\ &\leqslant\, a_B, \end{aligned}$$

thus proving the translation boundedness of μ. □

Remark 4.9.22. We note that a translation bounded measure μ is zero if and only if $f * \mu = 0$ for all $f \in C_{\mathsf{c}}(G)$. If μ is a positive[10] measure and $f \in C_{\mathsf{c}}(G)$ is non-negative, then $f * \mu$ is also a non-negative function. This is a test for the positivity of μ: Indeed, μ is a positive measure if and only if $f * \mu$ is a non-negative function for all non-negative $f \in C_{\mathsf{c}}(G)$. This is easy to see by decomposing μ into its positive, negative, and imaginary parts. $\Diamond$

Theorem 4.9.23 ([1, Thm. 2.5])**.** *Let μ be a Fourier transformable measure. Then, $\widehat{\mu}$ is translation bounded, that is, $\widehat{\mu} \in \mathcal{M}^{\infty}(\widehat{G})$.*

Proof. Due to the transformability of μ, the mapping $f \mapsto \widehat{f}$ is a linear mapping from $C_{\mathsf{c}}(G)$ to $L^2(\widehat{\mu})$. Let K be a symmetric, compact subset of G, so $K = -K$, and let $C(G, K)$ be the space of continuous functions on G whose support is in K. We check that the Fourier transform on $C(G, K)$ with the sup-norm into $L^2(\widehat{\mu})$ is continuous by showing that its graph is closed. For this purpose, let $\{f_n\}$ be a sequence of functions in $C(G, K)$ and suppose that $\{f_n\} \longrightarrow f$ in the sup-norm. At the same time, assume that $\{\widehat{f_n}\} \longrightarrow g$ in $L^2(\widehat{\mu})$. We need to prove that $g = \widehat{f}$ in $L^2(\widehat{\mu})$.

Suppose not; then, there is a compact set $B \subseteq \widehat{G}$ with

$$\left(\int_B \left| \widehat{f} - g \right|^2 \mathrm{d}|\widehat{\mu}| \right)^{\frac{1}{2}} > \varepsilon > 0 \tag{4.9.8}$$

for some positive ε. There is an n_0 so that, for all $n > n_0$,

$$\left\| \widehat{f_n} - \widehat{f} \right\|_{\infty} \leqslant \frac{\varepsilon}{2|\widehat{\mu}|(B)^{1/2} + 1} ,$$

from which we have

$$\left(\int_B \left| \widehat{f_n} - \widehat{f} \right|^2 \mathrm{d}|\widehat{\mu}| \right)^{\frac{1}{2}} < \frac{\varepsilon}{2}.$$

Possibly modifying n_0, we may also assume that

$$\left(\int_B \left| \widehat{f_n} - g \right|^2 \mathrm{d}|\widehat{\mu}| \right)^{\frac{1}{2}} \leqslant \left(\int_{\widehat{G}} \left| \widehat{f_n} - g \right|^2 \mathrm{d}|\widehat{\mu}| \right)^{\frac{1}{2}} < \frac{\varepsilon}{2}.$$

Together, these contradict Eq. (4.9.8). This shows the continuity. Thus, there exists a constant k_K so that, for all $f \in C(G, K)$, we have

$$\left(\int_{\widehat{G}} \left| \widehat{f} \right|^2 \mathrm{d}|\widehat{\mu}| \right)^{\frac{1}{2}} \leqslant k_K \|f\|_{\infty}.$$

[10]Note that, in line with common practice in the literature, the term 'positive' in conjunction with measures includes the zero measure, while we use the term 'non-negative' in the context of functions. A non-negative function is called positive if it is > 0 somewhere, while a strictly positive function is > 0 everywhere.

Since $K = -K$, this relation also holds when we use the inverse transform $\check{f}$ instead of $\widehat{f}$. Furthermore, multiplication by characters is well-behaved: If $\chi \in \widehat{G}$, we also have

$$\left(\int_{\widehat{G}} \bigl| T_\chi \check{f} \bigr|^2 \, \mathrm{d}|\widehat{\mu}| \right)^{\frac{1}{2}} = \left(\int_{\widehat{G}} \bigl| \widetilde{\chi f} \bigr|^2 \, \mathrm{d}|\widehat{\mu}| \right)^{\frac{1}{2}} \leqslant k_K \| f \|_\infty .$$

Now, let $A \subseteq \widehat{G}$ be an arbitrary compact set. Choose $g \in C_{\mathsf{c}}(G)$ so that $\check{g}(\psi) \geqslant 1$ on A (see Corollary 4.9.12) and let $K := \mathrm{supp}(g) \cup \mathrm{supp}(g^\dagger)$. Then, for all $\chi \in \widehat{G}$, we have

$$|\widehat{\mu}|(\chi + A) \leqslant \int_{\widehat{G}} |\check{g}(\psi - \chi)|^2 \, \mathrm{d}|\widehat{\mu}|(\psi) = \int_{\widehat{G}} |T_\chi \check{g}|^2 \, \mathrm{d}|\widehat{\mu}| \leqslant k_K^2 \| g \|_\infty^2 ,$$

and this is the desired translation boundedness. □

Lemma 4.9.24 ([1, Prop. 2.3])**.** *Let $\mu \in \mathcal{M}^\infty(G)$ be Fourier transformable and let $g \in \mathcal{K}_2(G)$. Then, $\widehat{g}\widehat{\mu}$ is a finite measure and its Fourier transform is $(g * \mu)^\dagger$, that is*

$$(g * \mu)(-x) = \widehat{\widehat{g}\widehat{\mu}}(x).$$

Proof. Since $g \in \mathcal{K}_2(G)$, one has $\widehat{g} \in L^1(\widehat{\mu}) = L^1(|\widehat{\mu}|)$ and

$$\bigl| \widehat{g}\widehat{\mu} \bigr|(\widehat{G}) = \int_{\widehat{G}} |\widehat{g}(\chi)| \, \mathrm{d}|\widehat{\mu}|(\chi) < \infty .$$

As $g \in C_{\mathsf{c}}(G)$ and μ is translation bounded, the convolution $g * \mu$ makes sense, and from $g \in \mathcal{K}_2(G)$ we have $T_x g^\dagger \in \mathcal{K}_2(G)$ for all $x \in G$.

Recalling that $\widehat{g}\widehat{\mu}$ is a finite measure, we have

$$\begin{aligned} (g * \mu)(x) &= \langle \mu, T_x g^\dagger \rangle = \bigl\langle \widehat{\mu}, \widetilde{T_x g^\dagger} \bigr\rangle = \int_{\widehat{G}} \widetilde{T_x g^\dagger} \, \mathrm{d}\widehat{\mu} \\ &= \int_{\widehat{G}} x(\chi) \, \check{g^\dagger}(\chi) \, \mathrm{d}\widehat{\mu}(\chi) = \int_{\widehat{G}} x(\chi) \, \widehat{g}(\chi) \, \mathrm{d}\widehat{\mu}(\chi) \\ &= \int_{\widehat{G}} \overline{(-x)(\chi)} \, \widehat{g}(\chi) \, \mathrm{d}\widehat{\mu}(\chi) = \widehat{\widehat{g}\widehat{\mu}}(-x), \end{aligned}$$

which completes the argument. □

Proposition 4.9.25 ([1, Prop. 2.4])**.** *Let μ be a Fourier transformable Radon measure on G and let $g \in \mathcal{K}_2(G)$. Then, $\widehat{g}$ and $\widehat{\mu}$ are convolvable as measures, and*

$$\widehat{g} * \widehat{\mu} = \widehat{g\mu}.$$

Proof. As $g \in \mathcal{K}_2(G)$, it follows that $\widehat{g} \in L^1(\widehat{\mu})$. By Corollary 4.9.20 and Theorem 4.9.23, $\widehat{g}$ and $\widehat{\mu}$ are convolvable as measures. Using Lemma 4.9.6, $\overline{\chi} g \in \mathcal{K}_2(G)$, and we have $\widetilde{\overline{\chi} g} \in L^1(\widehat{\mu})$, with $\langle \mu, \overline{\chi} g \rangle = \bigl\langle \widehat{\mu}, \widetilde{\overline{\chi} g} \bigr\rangle$. Thus,

$$\int_G \overline{\chi}(x) g(x) \, \mathrm{d}\mu(x) = \int_{\widehat{G}} \widehat{g}(\chi - \psi) \, \mathrm{d}\widehat{\mu}(\psi).$$

The left-hand side of this equation is the Fourier transform of the finite measure $g\mu$ evaluated at χ. To complete the proof, we will show that the convolution $\widehat{g} * \widehat{\mu}$ of measures is the absolutely continuous measure with Radon–Nikodym density J given by

$$J(\chi) \,=\, \int_{\widehat{G}} \widehat{g}(\chi - \psi)\, \mathrm{d}\widehat{\mu}(\psi).$$

Indeed, for all $h \in C_{\mathsf{c}}(\widehat{G})$, we have

$$\begin{aligned}
\int_{\widehat{G}} h(\chi)\, \mathrm{d}(\widehat{g} * \widehat{\mu})(\chi) \,&=\, \int_{\widehat{G}} \int_{\widehat{G}} h(\chi + \psi)\, \mathrm{d}\widehat{g}(\chi)\, \mathrm{d}\widehat{\mu}(\psi) \\
&=\, \int_{\widehat{G}} \int_{\widehat{G}} h(\chi + \psi)\, \widehat{g}(\chi)\, \mathrm{d}\chi\, \mathrm{d}\widehat{\mu}(\psi) \\
&=\, \int_{\widehat{G}} \int_{\widehat{G}} h(\varphi)\, \widehat{g}(\varphi - \psi)\, \mathrm{d}\varphi\, \mathrm{d}\widehat{\mu}(\psi) \\
&=\, \int_{\widehat{G}} \int_{\widehat{G}} h(\varphi)\, \widehat{g}(\varphi - \psi)\, \mathrm{d}\widehat{\mu}(\psi)\, \mathrm{d}\varphi \\
&=\, \int_{\widehat{G}} h(\varphi) \int_{\widehat{G}} \widehat{g}(\varphi - \psi)\, \mathrm{d}\widehat{\mu}(\psi)\, \mathrm{d}\varphi \,=\, \int_{\widehat{G}} h(\varphi)\, J(\varphi)\, \mathrm{d}\varphi,
\end{aligned}$$

where Fubini's theorem was used in the penultimate line. □

Lemma 4.9.26 ([1, Thm. 3.1])**.** *Let μ be a Fourier transformable Radon measure and let κ be a finite measure. If κ and μ are convolvable, then $\kappa * \mu$ is a Fourier transformable measure and*

$$\widehat{\kappa * \mu} \,=\, \widehat{\kappa}\widehat{\mu}.$$

Proof. Since $\widehat{\kappa}$ is a uniformly continuous bounded function and $\widehat{\mu}$ is a translation bounded measure, the product $\widehat{\kappa}\widehat{\mu}$ is a well-defined Radon measure.

Let $f \in \mathcal{K}_2(G)$. Then, by the definition of the convolution, we have

$$\langle \kappa * \mu, f \rangle \,=\, \int_G \int_G f(s + t)\, \mathrm{d}\mu(t)\, \mathrm{d}\kappa(s).$$

Let T_{-s} be the usual translation operator, so $\big(T_{-s} f\big)(t) = f(t+s)$. Then, $T_{-s} f \in \mathcal{K}_2(G)$ and, as μ is Fourier transformable, we have

$$\begin{aligned}
\int_G f(s + t)\, \mathrm{d}\mu(t) \,&=\, \langle \mu, T_{-s} f \rangle \,=\, \langle \widehat{\mu}, \widetilde{T_{-s} f} \rangle \\
&=\, \int_{\widehat{G}} \big(\widetilde{T_{-s} f}\big)(\chi)\, \mathrm{d}\widehat{\mu}(\chi) \,=\, \int_{\widehat{G}} \overline{\chi(s)}\, \check{f}(\chi)\, \mathrm{d}\widehat{\mu}(\chi).
\end{aligned}$$

This gives us the relation

$$\langle \kappa * \mu, f \rangle \,=\, \int_G \left(\int_{\widehat{G}} \overline{\chi(s)}\, \check{f}(\chi)\, \mathrm{d}\widehat{\mu}(\chi) \right) \mathrm{d}\kappa(s). \tag{4.9.9}$$

From the definition of the Fourier transformability of μ, we know by Proposition 4.9.9 that $\check{f} \in L^1(\widehat{\mu})$. Since $\widehat{\kappa}(\chi)$ is uniformly continuous and bounded, we also have

$$\check{f}\widehat{\kappa} \in L^1(\widehat{\mu}) \quad \text{and} \quad \check{f} \in L^1(\widehat{\mu}\widehat{\kappa}).$$

From $\check{f} \in L^1(\widehat{\mu})$ and the fact that κ is a finite measure, using Fubini's theorem, we get

$$\begin{aligned}\langle \widehat{\kappa}\widehat{\mu}, \check{f} \rangle &= \int_{\widehat{G}} \check{f}(\chi)\, \widehat{\kappa}(\chi)\, \mathrm{d}\widehat{\mu}(\chi) = \int_{\widehat{G}} \check{f}(\chi) \left(\int_G \overline{\chi(s)}\, \mathrm{d}\kappa(s) \right) \mathrm{d}\widehat{\mu}(\chi) \\ &= \int_G \int_{\widehat{G}} \check{f}(\chi)\, \overline{\chi(s)}\, \mathrm{d}\widehat{\mu}(\chi)\, \mathrm{d}\kappa(s).\end{aligned}$$

Finally, using Eq. (4.9.9), we see that, for all functions $f \in \mathcal{K}_2(G)$, we have $\check{f} \in L^1(\widehat{\mu}\widehat{\kappa})$ and

$$\langle \widehat{\kappa}\widehat{\mu}, \check{f} \rangle = \langle \kappa * \mu, f \rangle,$$

which proves our claim. □

Corollary 4.9.27. *Let μ be a twice Fourier transformable measure and let $f \in \mathcal{K}_2(G)$. Then, $\widehat{f} * \widehat{\mu}$ is Fourier transformable and its Fourier transform is given by $\widehat{\widehat{\mu}}\widehat{\widehat{f}}$.*

Proof. Note that $\widehat{\mu}$ is translation bounded and that $\widehat{f} \in L^1(\widehat{\mu})$, so $\widehat{f}$ and $\widehat{\mu}$ are convolvable by Corollary 4.9.20. The claim is now an immediate consequence of Proposition 4.9.26. □

We are now able to prove the following important result.

Theorem 4.9.28 ([1, Thm. 3.4])**.** *Let μ be a Fourier transformable Radon measure and assume that $\widehat{\mu}$ is also Fourier transformable. Then,*

$$\widehat{\widehat{\mu}} = \mu^{\dagger}.$$

Proof. Let $g \in \mathcal{K}_2(G)$. Then, $\widehat{g} \in L^1(\widehat{\mu})$ and $\widehat{\widehat{g}} = g^{\dagger}$ by Proposition 4.8.1, and we can consider $g^{\dagger}$ as an element of $K_2(\widehat{\widehat{G}})$. The argument ought to run like this:

$$\langle \widehat{\widehat{\mu}}, g^{\dagger} \rangle = \langle \widehat{\widehat{\mu}}, \widehat{\widehat{g}} \rangle = \langle \widehat{\mu}, \breve{g} \rangle = \langle \mu, g \rangle = \langle \mu^{\dagger}, g^{\dagger} \rangle,$$

so $\widehat{\widehat{\mu}}$ and $\mu^{\dagger}$ agree on the dense subspace $\mathcal{K}_2(G) \subseteq C_{\mathsf{c}}(G)$, and then $\widehat{\widehat{\mu}} = \mu^{\dagger}$. The trouble lies at the second equality. We are using the fact that $\widehat{\mu}$ is transformable. But the function $\breve{g}$ is not in $\mathcal{K}_2(G)$, as we would need it to be in order to apply the definition of the Fourier transform. The rest of the argument thus is about proving the second equality.

Define

$$I(\chi) := \int_{\widehat{G}} \chi(x)\, \widehat{\widehat{g}}(x)\, \mathrm{d}\widehat{\widehat{\mu}}(x),$$

which exists for all $\chi \in \widehat{G}$ and is a continuous function in χ. Let $f \in \mathcal{K}_2(\widehat{G})$. Then, using Corollary 4.9.27, we have

$$\begin{aligned}\bigl\langle \widehat{g} * \widehat{\mu}, f \bigr\rangle &= \Bigl\langle \widehat{\widehat{g}}\widehat{\widehat{\mu}}, \check{f} \Bigr\rangle = \int_G \check{f}(x)\, \widehat{\widehat{g}}(x)\, \mathrm{d}\widehat{\widehat{\mu}}(x) \\ &= \int_G \Bigl(\int_{\widehat{G}} f(\chi)\, \chi(x)\, \mathrm{d}\chi \Bigr) \widehat{\widehat{g}}(x)\, \mathrm{d}\widehat{\widehat{\mu}}(x) \\ &= \int_{\widehat{G}} \int_G f(\chi)\, \chi(x)\, \widehat{\widehat{g}}(x)\, \mathrm{d}\widehat{\widehat{\mu}}(x)\, \mathrm{d}\chi \,=\, \langle I, f \rangle .\end{aligned}$$

Thus, as measures, $\widehat{g} * \widehat{\mu}$ and I agree on the dense subspace $\mathcal{K}_2(\widehat{G}) \subseteq C_{\mathsf{c}}(\widehat{G})$, and hence are equal as measures. Since, as functions, both $\widehat{g} * \widehat{\mu}$ and I are continuous, they are equal everywhere. In particular, they are equal at the trivial character $\chi \equiv 1$, and thus

$$\bigl\langle \widehat{\widehat{\mu}}, \widehat{\widehat{g}} \bigr\rangle \,=\, I(1) \,=\, \bigl(\widehat{g} * \widehat{\mu}\bigr)(1) \,=\, \langle \widehat{\mu}, \widehat{g}^{\dagger} \rangle \,=\, \langle \widehat{\mu}, \check{g} \rangle .$$

This proves that the second equality is indeed true, which completes the proof of the theorem. □

Double Fourier transformability is a delicate issue. Here are some recent results [39].

Lemma 4.9.29. *Let μ be a Fourier transformable Radon measure on G and let $g \in \mathcal{K}_2(\widehat{G})$. Then, the measure $\widehat{g}\mu$ is Fourier transformable, and its Fourier transform is $g^{\dagger} * \widehat{\mu}$.*

Proof. Let $f \in \mathcal{K}_2(G)$. By Proposition 4.9.25, $\widehat{f}$ and $\widehat{\mu}$ are convolvable as measures and $\widehat{\mu} * \widehat{f}$ is the Fourier transform of the finite measure $f\mu$. Moreover, by Lemma 4.9.15, the measure $\widehat{\mu} * \widehat{f}$ is also Fourier transformable, with

$$\widehat{\widehat{\mu} * \widehat{f}} = (f\mu)^{\dagger}.$$

As $g \in \mathcal{K}_2(\widehat{G})$, the definition of the Fourier transform implies

$$\bigl\langle \widehat{\mu} * \widehat{f}, g \bigr\rangle \,=\, \bigl\langle (f\mu)^{\dagger}, \check{g} \bigr\rangle \,=\, \bigl\langle f\mu, \check{g^{\dagger}} \bigr\rangle \,=\, \bigl\langle \check{g^{\dagger}}\mu, f \bigr\rangle .$$

Next, $\widehat{\mu}$ is translation bounded by Theorem 4.9.23. Now, Theorem 4.9.21 implies that $g^{\dagger} * \widehat{\mu} \in C_{\mathsf{u}}(G)$. Since $\check{f} \in L^1(\widehat{\mu})$, we also have $\check{f} \in L^1(g^{\dagger} * \widehat{\mu})$.

By the definition of the convolution $\widehat{\mu} * \widehat{f}$, we obtain

$$\begin{aligned}\bigl\langle \widehat{\mu} * \widehat{f}, g \bigr\rangle &= \int_{\widehat{G}} \int_{\widehat{G}} g(\chi + \psi)\, \widehat{f}(\psi)\, \mathrm{d}\widehat{\mu}(\chi)\, \mathrm{d}\psi \\ &= \int_{\widehat{G}} \bigl(g^{\dagger} * \widehat{\mu}\bigr)(-\psi)\, \widehat{f}(\psi)\, \mathrm{d}\psi \,=\, \bigl\langle g^{\dagger} * \widehat{\mu}, \check{\widehat{f}} \bigr\rangle .\end{aligned}$$

We therefore have

$$\bigl\langle g^{\dagger} * \widehat{\mu}, \check{f} \bigr\rangle \,=\, \bigl\langle \check{g^{\dagger}}\mu, f \bigr\rangle \,=\, \bigl\langle \widehat{g}\mu, f \bigr\rangle ,$$

which proves the claim. □

Theorem 4.9.30 ([39, Thm. 3.10])**.** *Let $\mu \in \mathcal{M}^\infty(G)$ be Fourier transformable and let $\widehat{\mu}$ be its Fourier transform. Then, $\widehat{\mu}$ is Fourier transformable if and only if $\widehat{\mathcal{K}_2}(\widehat{G}) \subseteq L^1(\mu)$.*

Proof.

$\Longrightarrow$: Let $\widehat{\mu}$ be Fourier transformable. Then, by Theorem 4.9.28, we have

$$\widehat{\widehat{\mu}} = \mu^\dagger.$$

Therefore, by the definition of the Fourier transformability of $\widehat{\mu}$, we have $\check{f} \in L^1(\mu^\dagger)$ for all functions $f \in \mathcal{K}_2(\widehat{G})$. This is equivalent to $\widehat{f} \in L^1(\mu)$ for all $f \in \mathcal{K}_2(\widehat{G})$.

$\Longleftarrow$: Let $g \in \mathcal{K}_2(\widehat{G})$. By assumption, we have $\check{g} \in L^1(\mu)$. By Lemma 4.9.29, the measure $\widehat{g}\mu$ is Fourier transformable, and its Fourier transform is $g^\dagger * \widehat{\mu}$.

Now, by our assumption, the measure $\widecheck{g^\dagger}\mu$ is finite. Let

$$I(\chi) = \int_G \overline{\chi(t)}\, \widehat{g}(t)\, \mathrm{d}\mu(t)$$

be its Fourier transform as a finite measure; see Proposition 4.8.2. Then, by Lemma 4.9.14, the measure $\widecheck{g^\dagger}\mu$ is Fourier transformable and its Fourier transform is $I\theta_{\widehat{G}}$. Therefore, both $I\theta_{\widehat{G}}$ and $g^\dagger * \widehat{\mu}$ are Fourier transforms of $\widecheck{g^\dagger}\mu$, and hence, by Theorem 4.9.13, they are equal as measures.

Finally, I is a continuous function on $\widehat{G}$, and the measure $\widehat{\mu}$ is translation bounded by Theorem 4.9.23. Consequently, by Theorem 4.9.21, the function $g^\dagger * \widehat{\mu}$ is also continuous. Since both I and $g^\dagger * \widehat{\mu}$ are continuous, and equal as measures, they are equal as functions. In particular,

$$\langle \widehat{\mu}, g \rangle = \big(g^\dagger * \widehat{\mu}\big)(1) = I(1) = \langle \mu, \widehat{g} \rangle = \langle \mu^\dagger, \check{g} \rangle.$$

This shows that $\widehat{\mu}$ is Fourier transformable, with Fourier transform $\mu^\dagger$. □

For $G = \mathbb{R}^d$, it was shown in [39] that the integrability condition in Theorem 4.9.30 can be replaced by translation boundedness of μ.

As an immediate consequence, we get a type of domination condition for double Fourier transformability.

Corollary 4.9.31. *Let $\mu \in \mathcal{M}^\infty(G)$ and $\nu \in \mathcal{M}^\infty(\widehat{G})$ be Fourier transformable. If $|\mu| \leqslant |\widehat{\nu}|$, the measure $\widehat{\mu}$ is Fourier transformable as well.*

Proof. Let $g \in \mathcal{K}_2(\widehat{G})$. Then, by the Fourier transformability of ν, we have $\widehat{g} \in L^1(\widehat{\nu})$. Since $|\mu| \leqslant |\widehat{\nu}|$, we have

$$\big\langle\, |\mu|\,, |\widehat{g}|\,\big\rangle \leqslant \big\langle\, |\widehat{\nu}|\,, |\widehat{g}|\,\big\rangle < \infty,$$

showing that $\widehat{g} \in L^1(\mu)$ and hence $\widehat{\mathcal{K}_2}(\widehat{G}) \subseteq L^1(\mu)$. The claim now follows from Theorem 4.9.30. □

We complete this section by showing that every translation bounded, Fourier transformable measure with Meyer set support is twice Fourier transformable. For the definitions of Meyer sets and cut and project schemes in arbitrary LCAGs, we refer the reader to Chapter 5 in this volume [46]. These non-trivial concepts are needed for the remainder of this section; see [AO1] for general background.

Theorem 4.9.32 ([39, Thm. 5.9])**.** *Let μ be a translation bounded, Fourier transformable measure on G. If $\mathrm{supp}(\mu)$ is a subset of a Meyer set, then $\widehat{\mu}$ is Fourier transformable.*

Proof. Let $\varLambda$ be a Meyer set such that $\mathrm{supp}(\mu) \subseteq \varLambda$, so

$$\mu \,=\, \sum_{x\in\varLambda} w_x \delta_x ,$$

where $w_x \in \mathbb{C}$ for all $x \in \varLambda$. Note that, since the support of μ might not be relatively dense, we need to allow for w_x to be 0 for some x.

Since μ is translation bounded, there exists a constant C such that

$$|w_x| \leqslant C \quad \text{for all } x \in \varLambda.$$

Since $\varLambda$ is a Meyer set, there exists a *cut and project scheme* $(G, H, \mathcal{L})$ and a compact set $W \subseteq H$ such that

$$\varLambda \,\subseteq\, \curlywedge(W);$$

see Theorem 5.7.8 on page 310. By Lemma 4.9.12, there exists a function $g \in \mathcal{K}_2(\widehat{H})$ such that $\widehat{g} \geqslant 1_W$.

Now, let us consider the dual cut and project scheme $(\widehat{G}, \widehat{H}, \mathcal{L}^0)$ of Definition 5.6.13 from page 303, and set

$$\omega \,:=\, \sum_{(\chi,\psi)\in\mathcal{L}^0} g(\psi)\, \delta_\chi .$$

Then, by Theorem 5.10.6 from page 334, if γ is an autocorrelation of ω then

$$\widehat{\gamma} \,=\, \sum_{(x,x^\star)\in\mathcal{L}} \widehat{g}(x^\star)\, \delta_x .$$

We thus have

$$\widehat{C\gamma} \,=\, C\widehat{\gamma} \,=\, \sum_{(x,x^\star)\in\mathcal{L}} C\, \widehat{g}(x^\star)\, \delta_x \,\geqslant\, \sum_{x\in\curlywedge(W)} C\, \delta_x \,\geqslant\, |\mu| ,$$

and the claim now follows from Corollary 4.9.31. □

4.10. Almost periodic measures

Note. *Throughout this section, $\{f_\alpha\} \subset C_{\mathsf{c}}(G)$ will denote an approximate identity for $(C_{\mathsf{u}}(G), *)$; see Remark* 4.7.6 *as well as Proposition* 4.7.7.

4.10.1. Introducing $\mathcal{WAP}(G)$, $\mathcal{SAP}(G)$ and $\mathcal{WAP}_0(G)$

Definition 4.10.1. A measure μ is called *strongly*, *weakly*, or *null weakly almost periodic* if, for all $f \in C_{\mathsf{c}}(G)$, the function $f * \mu$ is a strongly, weakly, or null weakly almost periodic function, respectively. We will denote by $\mathcal{SAP}(G)$, $\mathcal{WAP}(G)$, and $\mathcal{WAP}_0(G)$ the spaces of strongly, weakly and null weakly almost periodic measures, so

$$\begin{aligned}
\mathcal{SAP}(G) &:= \big\{\mu \in \mathcal{M}^\infty(G) : \mu * f \in \mathrm{SAP}(G) \text{ for all } f \in C_{\mathsf{c}}(G)\big\},\\
\mathcal{WAP}(G) &:= \big\{\mu \in \mathcal{M}^\infty(G) : \mu * f \in \mathrm{WAP}(G) \text{ for all } f \in C_{\mathsf{c}}(G)\big\},\\
\mathcal{WAP}_0(G) &:= \big\{\mu \in \mathcal{M}^\infty(G) : \mu * f \in \mathrm{WAP}_0(G) \text{ for all } f \in C_{\mathsf{c}}(G)\big\}.
\end{aligned}$$

Obviously, $\mathcal{SAP}(G)$ and $\mathcal{WAP}_0(G)$ are subspaces of $\mathcal{WAP}(G)$.

Remark 4.10.2. Since $\mathrm{SAP}(G)$, $\mathrm{WAP}(G)$ and $\mathrm{WAP}_0(G)$ are closed in the strong topology of $C_{\mathsf{u}}(G)$ (see Proposition 4.3.4 and Definition 4.7.1), and since the mean is continuous, we conclude that the spaces $\mathcal{SAP}(G)$, $\mathcal{WAP}(G)$ and $\mathcal{WAP}_0(G)$ are closed in the sense that, if $\{\mu_\alpha\} \subset \mathcal{M}^\infty(G)$ and if a measure $\mu \in \mathcal{M}^\infty(G)$ exists with

$$\lim_\alpha (\mu_\alpha * f) = \mu * f \quad \text{for all } f \in C_{\mathsf{c}}(G), \tag{4.10.1}$$

one has

(i) $\mu \in \mathcal{SAP}(G)$ if $\mu_\alpha \in \mathcal{SAP}(G)$ for all α;
(ii) $\mu \in \mathcal{WAP}(G)$ if $\mu_\alpha \in \mathcal{WAP}(G)$ for all α;
(iii) $\mu \in \mathcal{WAP}_0(G)$ if $\mu_\alpha \in \mathcal{WAP}_0(G)$ for all α.

In [19], the authors use this observation to introduce a topology on $\mathcal{M}^\infty(G)$, defining convergence by Eq. (4.10.1). ◊

Proposition 4.10.3. *For $\mu \in \mathcal{M}^\infty(G)$, one has*

$$\mu \in \left\{\begin{matrix}\mathcal{SAP}(G)\\ \mathcal{WAP}(G)\\ \mathcal{WAP}_0(G)\end{matrix}\right\} \iff \mu * f * g \in \left\{\begin{matrix}\mathrm{SAP}(G)\\ \mathrm{WAP}(G)\\ \mathrm{WAP}_0(G)\end{matrix}\right\} \quad \begin{matrix}\text{for all}\\ f, g \in C_{\mathsf{c}}(G).\end{matrix}$$

Proof. If $f, g \in C_{\mathsf{c}}(G)$ and $\mu \in \mathcal{SAP}(G)$, one has $f * g \in C_{\mathsf{c}}(G)$ together with $\mu * f * g \in \mathrm{SAP}(G)$. Conversely, replacing g by elements of the approximate identity $\{f_\alpha\}$, we have $\{\mu * f * f_\alpha\} \subset \mathrm{SAP}(G)$ and thus

$$\mu * f = \lim_\alpha \big(\mu * f * f_\alpha\big) \in \mathrm{SAP}(G),$$

since the latter is closed in the strong topology by Proposition 4.3.4.

This argument effectively repeats for $\mathrm{WAP}(G)$ and $\mathrm{WAP}_0(G)$, recalling from page 230 that $\mathrm{WAP}_0(G)$ is closed. □

Theorem 4.10.4. *If $\mu \in \mathcal{M}^\infty(G)$ is transformable, one has $\mu \in \mathcal{WAP}(G)$.*

Proof. Let $g \in \mathcal{K}_2(G)$. By Lemma 4.9.24, $\widehat{g}\widehat{\mu}$ is a finite measure and $g * \mu$ is its inverse Fourier transform. Therefore, by Lemma 4.8.6, it is in $\mathrm{WAP}(G)$. By Proposition 4.10.3, $\mu \in \mathcal{WAP}(G)$. □

The following proposition shows that almost periodicity is compatible with the natural embedding $C_{\mathsf{u}}(G) \hookrightarrow \mathcal{M}^\infty(G)$ defined by $f \mapsto f\theta_G$.

Proposition 4.10.5. *For $f \in C_{\mathsf{u}}(G)$, the following properties hold,*

(i) $f \in \mathrm{SAP}(G) \iff f\theta_G \in \mathcal{SAP}(G)$;

(ii) $f \in \mathrm{WAP}(G) \iff f\theta_G \in \mathcal{WAP}(G)$;

(iii) $f \in \mathrm{WAP}_0(G) \iff f\theta_G \in \mathcal{WAP}_0(G)$.

Proof. In the '⇒' direction, parts (i) and (ii) were proved in Proposition 4.5.10.

For claim (i) in the '⇐' direction, suppose that $f\theta_G$ is a strongly almost periodic measure. Then, for all α, $f * f_\alpha$ is a strongly almost periodic function. We therefore know that $f = \lim_\alpha (f * f_\alpha)$ lies in $(C_{\mathsf{u}}(G), \|.\|_\infty)$, while $\mathrm{SAP}(G)$ is closed in $(C_{\mathsf{u}}(G), \|.\|_\infty)$ by Proposition 4.3.4. Hence, f is a strongly almost periodic function. This argument works the same way for the weakly almost periodic case.

Claim (iii): Let $f \in \mathrm{WAP}_0(G)$, and let $g \in C_{\mathsf{c}}(G)$ be arbitrary. Then, $f * g \in \mathrm{WAP}(G)$ by Proposition 4.5.10 and $M(|f|) = 0$. Since $\mathrm{WAP}(G)$ is closed under taking absolute values of functions (by Proposition 4.3.11), we conclude that $|f|$ and $|f * g|$ are in $\mathrm{WAP}(G)$ and that $|f * g| \leqslant |f| * |g|$. Then, by Proposition 4.5.10,

$$0 \leqslant M(|f * g|) \leqslant M(|f| * |g|) = M(|f|) \int_G |g| \, \mathrm{d}\theta_G = 0,$$

wherefore $f * g \in \mathrm{WAP}_0(G)$. This happens for all $g \in C_{\mathsf{c}}(G)$, showing that $f\theta_G \in \mathcal{WAP}_0(G)$.

Conversely, let $f\theta_G \in \mathcal{WAP}_0(G)$. We get $f \in \mathrm{WAP}(G)$ by (ii) and $f * f_\alpha$ in $\mathrm{WAP}_0(G)$ by Eq. (4.9.7) and Definition 4.10.1. Thus, $M(|f * f_\alpha|) = 0$. Since $\{f_\alpha\}$ is an approximate identity, we obtain

$$|f| = \lim_\alpha |f * f_\alpha| \, ,$$

and, using the continuity of M in the $\|.\|_\infty$-norm, we find $M(|f|) = 0$, that is, $f \in \mathrm{WAP}_0(G)$. □

Lemma 4.10.6. *Let $\mu \in \mathcal{WAP}(G)$. Then, there exists a number $M(\mu)$, the mean of μ, such that*

$$M(\mu * f) \,=\, M(\mu)\, \theta_G(f) \quad \text{holds for all } f \in C_{\mathsf{c}}(G).$$

Moreover, $M(\mu^{\dagger}) = M(\mu)$.

Proof. Let $f, g \in C_{\mathsf{c}}(G)$ be arbitrary. Since $\mu * f, \mu * g \in \mathrm{WAP}(G)$, Proposition 4.5.10 implies

$$M(\mu * g)\, \theta_G(f) \,=\, M(\mu * f * g) \,=\, M(\mu * f)\, \theta_G(g).$$

Now, if we fix some $g \in C_{\mathsf{c}}(G)$ with $\int_G g \,\mathrm{d}\theta_G = 1$ and define

$$M(\mu) \,:=\, M(\mu * g),$$

we have, for all $f \in C_{\mathsf{c}}(G)$,

$$M(\mu * f) \,=\, M(\mu * f)\, \theta_G(g) \,=\, M(\mu * g)\, \theta_G(f) \,=\, M(\mu)\, \theta_G(f).$$

This shows the existence of the mean.

The last claim is rather obvious. Indeed, if $g \in C_{\mathsf{c}}(G)$ is fixed with $\int_G g \,\mathrm{d}\theta_G = 1$, one obtains

$$M(\mu) \,=\, M(\mu * g) \,=\, M\big((\mu * g)^{\dagger}\big) \,=\, M\big((\mu^{\dagger}) * (g^{\dagger})\big) \,=\, M(\mu^{\dagger})\, \theta_G(g^{\dagger}),$$

which completes the argument. □

Lemma 4.10.7. *If G admits a van Hove sequence $\{A_n\}$, then, for all measures $\mu \in \mathcal{WAP}(G)$, we have*

$$M(\mu) \,:=\, \lim_{n\to\infty} \frac{\mu(t + A_n)}{\theta_G(A_n)},$$

uniformly in $t \in G$.

Proof. Let $f \in C_{\mathsf{c}}(G)$ be such that $\theta_G(f) = 1$. Since $\mu * f \in \mathrm{WAP}(G)$, we have

$$M(\mu) \,=\, M(\mu * f) \,=\, \lim_{n\to\infty} \frac{\int_{t+A_n} (\mu * f)\, \mathrm{d}\theta_G}{\theta_G(A_n)},$$

uniformly in $t \in G$. If we prove that

$$\lim_{n\to\infty} \frac{\int_{t+A_n} (\mu * f)\, \mathrm{d}\theta_G \,-\, \mu(t + A_n) \int_G f \,\mathrm{d}\theta_G}{\theta_G(A_n)} \,=\, 0 \tag{4.10.2}$$

holds uniformly in $t \in G$, we establish the claim.

For this, we compare $(\mu * f)|_{t+A_n}$ with $\mu|_{t+A_n} * f$. If $K = -K \subset G$ is a compact set so that $\mathrm{supp}(f) \subseteq K$, a simple computation (remembering that μ is translation bounded and f has compact support) shows that the function $(\mu * f)|_{t+A_n} - \mu|_{t+A_n} * f$ vanishes outside $\partial^K(t + A_n)$ and is bounded (independently of n and t) inside $\partial^K(t + A_n)$ (refer to Eq. (4.1.3) for the

notation). Moreover, we have $\partial^K(t + A_n) = t + \partial^K A_n$ by the definition of the K-boundary. Therefore, the van Hove property implies

$$\lim_n \frac{\int_{t+A_n} (\mu * f)\,\mathrm{d}\theta_G - \int_G (\mu|_{t+A_n} * f)\,\mathrm{d}\theta_G}{\theta_G(A_n)}$$
$$= \lim_n \frac{\int_G \bigl((\mu * f)|_{t+A_n} - (\mu|_{t+A_n} * f)\bigr)\,\mathrm{d}\theta_G}{\theta_G(A_n)} = 0,$$

uniformly in $t \in G$.

We now show that $\int_G (\mu|_{t+A_n} * f)\,\mathrm{d}\theta_G = \mu(t + A_n) \int_G f\,\mathrm{d}\theta_G$. Since both $\mu|_{t+A_n}$ and f are compactly supported, and thus finite, we obtain

$$\begin{aligned}\int_G \bigl(\mu|_{t+A_n} * f\bigr)(x)\,\mathrm{d}\theta_G(x) &= \int_G \int_G f(x-y)\,\mathrm{d}\mu|_{t+A_n}(y)\,\mathrm{d}\theta_G(x)\\ &= \int_G \int_G f(x-y)\,\mathrm{d}\theta_G(x)\,\mathrm{d}\mu|_{t+A_n}(y)\\ &= \int_G \left(\int_G f\,\mathrm{d}\theta_G\right)\mathrm{d}\mu|_{t+A_n}(y)\\ &= \mu(t+A_n)\int_G f\,\mathrm{d}\theta_G,\end{aligned}$$

where we made use of Fubini's theorem in the second step. □

Definition 4.10.8. For a measure $\mu \in \mathcal{WAP}(G)$, the *strongly almost periodic* and *null weakly almost periodic components* of μ are the measures (see below) μ_{s} and μ_0 defined by

$$\mu_{\mathsf{s}}(f) := \bigl(\mu * f^\dagger\bigr)_{\mathsf{s}}(0) \quad \text{and} \quad \mu_0(f) := \bigl(\mu * f^\dagger\bigr)_0(0),$$

for all $f \in C_{\mathsf{c}}(G)$.

Lemma 4.10.9. *Let $\mu \in \mathcal{WAP}(G)$. Then, we have $\mu_{\mathsf{s}}, \mu_0 \in \mathcal{M}^\infty(G)$ and, for all $g \in C_{\mathsf{c}}(G)$,*

$$\mu_{\mathsf{s}} * g = (\mu * g)_{\mathsf{s}} \quad \textit{and} \quad \mu_0 * g = (\mu * g)_0.$$

Proof. Since convolution, reflection, the projections

$$P_{\mathsf{s}}\colon \mathrm{WAP}(G) \longrightarrow \mathrm{SAP}(G) \quad \text{and} \quad P_0\colon \mathrm{WAP}(G) \longrightarrow \mathrm{WAP}_0(G)$$

as well as evaluation at 0 are continuous linear mappings (see Remark 4.7.13), we see that μ_{s} and μ_0 are continuous linear mappings from $C_{\mathsf{c}}(G)$ into $\mathbb{C}$, and thus are measures. We have

$$\begin{aligned}\bigl(\mu_{\mathsf{s}} * g\bigr)(x) &= \mu_{\mathsf{s}}\bigl(T_x(g^\dagger)\bigr) = \bigl(\mu * (T_x g^\dagger)^\dagger\bigr)_{\mathsf{s}}(0) = \bigl(\mu * T_{-x} g\bigr)_{\mathsf{s}}(0)\\ &= \bigl(T_{-x}(\mu * g)\bigr)_{\mathsf{s}}(0) = (\mu * g)_{\mathsf{s}}(x),\end{aligned}$$

whence $\mu_{\mathsf{s}} * g = (\mu * g)_{\mathsf{s}}$.

Similarly, we obtain $\mu_0 * g = (\mu * g)_0$. In particular, for all $g \in C_c(G)$, we have $\mu_0 * g, \mu_s * g \in C_u(G)$, which shows that $\mu_s, \mu_0 \in \mathcal{M}^\infty(G)$; compare Proposition 4.9.21. □

We can now establish one of the cornerstones of the theory of almost periodic measures.

Theorem 4.10.10. *For any LCAG G, one has the Eberlein decomposition*

$$\mathcal{WAP}(G) = \mathcal{SAP}(G) \oplus \mathcal{WAP}_0(G).$$

More specifically, for any measure $\mu \in \mathcal{WAP}(G)$, we have $\mu = \mu_s + \mu_0$ with $\mu_s \in \mathcal{SAP}(G)$ and $\mu_0 \in \mathcal{WAP}_0(G)$. This decomposition into strongly and null weakly almost periodic parts is unique.

Proof. By Lemma 4.10.9, for all $g \in C_c(G)$, we have

$$\mu_s * g = (\mu * g)_s \in \mathrm{SAP}(G) \quad \text{and} \quad \mu_0 * g = (\mu * g)_0 \in \mathrm{WAP}_0(G).$$

Thus, by definition, $\mu_s \in \mathcal{SAP}(G)$ and $\mu_0 \in \mathcal{WAP}_0(G)$.

Moreover, since $\mu * g \in \mathrm{WAP}(G)$, we have

$$\mu * g = (\mu * g)_s + (\mu * g)_0 = \mu_s * g + \mu_0 * g = (\mu_s + \mu_0) * g,$$

which is true for all $g \in C_c(G)$, and hence

$$\mu = \mu_s + \mu_0.$$

Uniqueness of this decomposition is a direct consequence of Theorem 4.7.11 and Proposition 4.10.3. □

Proposition 4.10.11. *Let $\mu \in \mathcal{WAP}(G)$ be a positive measure. Then, μ_s is positive as well.*

Proof. Let $f \in C_c(G)$ be non-negative but arbitrary. Then, the function $\mu * f^\dagger \in \mathrm{WAP}(G)$ is non-negative, and, by Theorem 4.7.11, $\mu_s * f^\dagger = \big(\mu * f^\dagger\big)_s$ is non-negative as well. Thus, $\mu_s(f) = \big(\mu_s * f^\dagger\big)(0) \geqslant 0$ for all non-negative functions $f \in C_c(G)$. □

4.10.2. Fourier transforms in $\mathcal{WAP}(G)$

Theorem 4.10.12. *Let $\mu \in \mathcal{M}^\infty(G)$ be Fourier transformable. Then, μ_s and μ_0 are also Fourier transformable, and one has*

$$\widehat{\mu_s} = (\widehat{\mu})_{pp} \quad \textit{and} \quad \widehat{\mu_0} = (\widehat{\mu})_c.$$

Proof. Let $g \in \mathcal{K}_2(G)$. Since $\widehat{g} \in L^1(\widehat{\mu})$, we have $\widehat{g} \in L^1(\widehat{\mu}_{pp})$ as well as $\widehat{g} \in L^1(\widehat{\mu}_c)$. Consequently, the measures $\widehat{g}\widehat{\mu}$, $\widehat{g}\widehat{\mu}_{pp}$ and $\widehat{g}\widehat{\mu}_c$ are finite.

Then, by Lemma 4.9.24, we have

$$(g * \mu)^\dagger = \widehat{\widehat{g}\widehat{\mu}},$$

where, by Lemma 4.9.14, $\widehat{\widehat{g}\widehat{\mu}}$ can be interpreted both as the Fourier transform of finite measures and as the Fourier transform of functions. Moreover, by Theorem 4.10.4, $(g * \mu)^{\dagger} \in \mathrm{WAP}(G)$. In the remainder of this proof, we will always interpret the Fourier transform of a finite measure as a continuous function.

Now, $\widehat{g}\widehat{\mu}_{\mathsf{pp}}$ and $\widehat{g}\widehat{\mu}_{\mathsf{c}}$ are finite pure point respectively continuous measures. By Theorem 4.8.11, we get

$$\widehat{\widehat{g}\widehat{\mu}_{\mathsf{pp}}} \in \mathrm{SAP}(G) \quad \text{and} \quad \widehat{\widehat{g}\widehat{\mu}_{\mathsf{c}}} \in \mathrm{WAP}_0(G),$$

wherefore we have

$$(g * \mu)^{\dagger} \,=\, \widehat{\widehat{g}\widehat{\mu}} \,=\, \widehat{\widehat{g}\widehat{\mu}_{\mathsf{pp}}} + \widehat{\widehat{g}\widehat{\mu}_{\mathsf{c}}}.$$

Since $(g * \mu)^{\dagger} \in \mathrm{WAP}(G)$ as well as $\widehat{\widehat{g}\widehat{\mu}_{\mathsf{pp}}} \in \mathrm{SAP}(G)$ and $\widehat{\widehat{g}\widehat{\mu}_{\mathsf{c}}} \in \mathrm{WAP}_0(G)$, the uniqueness of the decomposition yields

$$\big((g * \mu)^{\dagger}\big)_{\mathsf{s}} \,=\, \widehat{\widehat{g}\widehat{\mu}_{\mathsf{pp}}} \quad \text{and} \quad \big((g * \mu)^{\dagger}\big)_{0} \,=\, \widehat{\widehat{g}\widehat{\mu}_{\mathsf{c}}}.$$

By Lemma 4.10.9, we have $\big((g*\mu)^{\dagger}\big)_{\mathsf{s}} = (g*\mu_{\mathsf{s}})^{\dagger}$ and $\big((g*\mu)^{\dagger}\big)_{0} = (g*\mu_0)^{\dagger}$, which shows that, as continuous functions, we have

$$(g * \mu_{\mathsf{s}})^{\dagger} \,=\, \widehat{\widehat{g}\widehat{\mu}_{\mathsf{pp}}} \quad \text{and} \quad (g * \mu_0)^{\dagger} \,=\, \widehat{\widehat{g}\widehat{\mu}_{\mathsf{c}}}.$$

Evaluating at 0, we get

$$\langle g^{\dagger}, \mu_{\mathsf{s}} \rangle \,=\, (g * \mu_{\mathsf{s}})^{\dagger}(0) \,=\, \widehat{\widehat{g}\widehat{\mu}_{\mathsf{pp}}}(0) \,=\, \langle \widehat{g}, \widehat{\mu}_{\mathsf{pp}} \rangle$$

and

$$\langle g^{\dagger}, \mu_0 \rangle \,=\, (g * \mu_0)^{\dagger}(0) \,=\, \widehat{\widehat{g}\widehat{\mu}_{\mathsf{c}}}(0) \,=\, \langle \widehat{g}, \widehat{\mu}_{\mathsf{c}} \rangle.$$

Therefore, for all $g \in \mathcal{K}_2(G)$, we have $\widehat{g} \in L^1(\widehat{\mu}_{\mathsf{pp}})$ and $\widehat{g} \in L^1(\widehat{\mu}_{\mathsf{c}})$, as well as

$$\langle g^{\dagger}, \mu_{\mathsf{s}} \rangle \,=\, \langle \widehat{g}, \widehat{\mu}_{\mathsf{pp}} \rangle \quad \text{and} \quad \langle g^{\dagger}, \mu_0 \rangle \,=\, \langle \widehat{g}, \widehat{\mu}_{\mathsf{c}} \rangle,$$

which proves the claim. □

One important consequence of Theorem 4.10.12 can be stated as follows.

Corollary 4.10.13. *Let $\mu \in \mathcal{M}^{\infty}(G)$ be Fourier transformable. Then, $\widehat{\mu}$ is a pure point measure if and only if $\mu \in \mathcal{SAP}(G)$, and $\widehat{\mu}$ is continuous if and only if $\mu \in \mathcal{WAP}_0(G)$.* □

For $G = \mathbb{R}^d$, the following result was proved by Hof in [22, 21], while a general proof via dynamical systems was given in [25]. For twice Fourier transformable measures, the result also follows from [19]. Below, we give a proof based on almost periodicity.

Theorem 4.10.14. *Let μ be a measure on G that is translation bounded and Fourier transformable. Then, for all $\chi \in \widehat{G}$, one has*

$$\widehat{\mu}(\{\chi\}) \,=\, M(\overline{\chi}\mu).$$

Moreover, if G admits a van Hove sequence $\{A_n\}$, we have

$$\widehat{\mu}(\{\chi\}) \,=\, \lim_{n\to\infty} \frac{\int_{A_n} \overline{\chi}(x)\,\mathrm{d}\mu(x)}{\theta_G(A_n)}.$$

Proof. Let $f \in \mathcal{K}_2(G)$. By Lemma 4.9.24, $\check{f}\widehat{\mu}$ is a finite measure. Then, by Lemma 4.8.7, we know that

$$\int_G f(t)\chi(t)\,\mathrm{d}\theta_G(t)\,\widehat{\mu}(\{\chi\}) \,=\, \big(\check{f}\widehat{\mu}\big)(\{\chi\}) \,=\, M\Big(\chi\,\widehat{\check{f}\widehat{\mu}}\Big) \,=\, M\big(\chi\cdot(f*\mu^{\dagger})\big).$$

Now, a simple calculation yields

$$\begin{aligned}\chi(t)\big(f*\mu^{\dagger}\big)(t) \,&=\, \chi(t)\int_G f(t-s)\,\mathrm{d}\mu^{\dagger}(s) \,=\, \int_G f(t-s)\,\chi(t-s)\,\chi(s)\,\mathrm{d}\mu^{\dagger}(s)\\ &=\int_G f(t-s)\,\chi(t-s)\,\mathrm{d}\big(\chi\mu^{\dagger}\big)(s) \,=\, \big((\chi f)*(\chi\mu^{\dagger})\big)(t).\end{aligned}$$

We therefore have

$$\begin{aligned}\int_G f(t)\,\chi(t)\,\mathrm{d}\theta_G(t)\,\widehat{\mu}(\{\chi\}) \,&=\, M\big((\chi f)*(\chi\mu^{\dagger})\big)\\ &=\, M(\chi\mu^{\dagger})\int_G f(t)\,\chi(t)\,\mathrm{d}\theta_G(t),\end{aligned}$$

where Lemma 4.10.7 was used in the last step.

Now, by choosing some $f \in \mathcal{K}_2(G)$ with $\int_G f(t)\chi(t)\,\mathrm{d}\theta_G(t) \neq 0$, we get

$$\widehat{\mu}\big(\{\chi\}\big) \,=\, M\big(\chi\mu^{\dagger}\big) \,=\, M\big(\overline{\chi}\mu\big),$$

which completes the proof. □

4.11. Positive definite measures

Finally, we come to the heart of the matter, the Fourier transformation of positive definite measures. Recall that diffraction is defined as the Fourier transform of the volume-averaged autocorrelation measure, which is always positive definite; see [AO1, Ch. 9]. The purpose of this section is to show that positive definite measures are indeed always Fourier transformable. Then, we also study the Fourier transform of measures that are both positive and positive definite.

Definition 4.11.1. A measure μ on G is *positive definite* if, for all functions $f \in C_{\mathsf{c}}(G)$, one has

$$\mu\big(f*\widetilde{f}\,\big) \,\geqslant\, 0.$$

Lemma 4.11.2. *A Radon measure μ on G is positive definite if and only if $\mu * f * \widetilde{f}$ is a continuous positive definite function for all $f \in C_{\mathsf{c}}(G)$.*

PROOF. Suppose that μ is a positive definite measure on G. For all functions $f \in C_{\mathsf{c}}(G)$, we have $\langle \mu, f\rangle = (\mu * f^{\dagger})(0)$.

Let $f, g \in C_{\mathsf{c}}(G)$. It is clear that $\mu * f * \widetilde{f}$ is continuous, and that

$$\begin{aligned}\bigl\langle \mu * f * \widetilde{f}, g * \widetilde{g}\bigr\rangle \;&=\; \bigl(\mu * f * \widetilde{f} * g^{\dagger} * \widetilde{g}^{\dagger}\bigr)(0) \;=\; \bigl(\mu * f * g^{\dagger} * \widetilde{f * g^{\dagger}}\bigr)(0)\\ &=\; \bigl\langle \mu \,, (f^{\dagger} * g) * \widetilde{f^{\dagger} * g}\bigr\rangle \;\geqslant\; 0.\end{aligned}$$

Let $\varepsilon > 0$, $x_1, \ldots, x_n \in G$ and $c_1, \ldots, c_n \in \mathbb{C}$. Since the pure point measure $\nu := \sum_j c_j \delta_{x_j}$ can be approximated, in the vague topology, by compactly supported functions, there exists a net of functions $\{h_\alpha\} \subset C_{\mathsf{c}}(G)$ so that

$$\bigl\langle \mu * f * \widetilde{f}, \nu * \widetilde{\nu}\bigr\rangle \;=\; \lim_{\alpha} \bigl\langle \mu * f * \widetilde{f}, h_\alpha * \widetilde{h_\alpha}\bigr\rangle \;\geqslant\; 0.$$

But, we also have

$$\bigl\langle \mu * f * \widetilde{f}, \nu * \widetilde{\nu}\bigr\rangle \;=\; \sum_{i,j} \bigl(\mu * f * \widetilde{f}\bigr)(x_i - x_j)\, c_i \overline{c_j},$$

wherefore $\mu * f * \widetilde{f}$ is positive definite.

In the converse direction, let $f \in C_{\mathsf{c}}(G)$. By assumption, $\mu * f^{\dagger} * \widetilde{f^{\dagger}}$ is positive definite, and since positive definite functions are always non-negative at 0, we have $\bigl(\mu * f^{\dagger} * \widetilde{f^{\dagger}}\bigr)(0) \geqslant 0$. Thus, $\bigl\langle \mu, f * \widetilde{f}\,\bigr\rangle \geqslant 0$. □

Lemma 4.11.3 ([5, Thm. 4.4])**.** *Any positive and positive definite Radon measure μ on G is translation bounded.*

PROOF. Let $K \subseteq G$ be a compact set and let $f \in C_{\mathsf{c}}(G)$ be chosen so that $f * \widetilde{f} \geqslant 1_K$. Then, $\mu * f * \widetilde{f}$ is positive definite by Lemma 4.11.2, and also a non-negative function. Consequently, as for all functions of this kind, we have $0 \leqslant \bigl(\mu * f * \widetilde{f}\bigr)(y) \leqslant \bigl(\mu * f * \widetilde{f}\bigr)(0)$. From this observation, it easily follows that

$$\|\mu\|_K \;\leqslant\; \bigl(\mu * f * \widetilde{f}\bigr)(0),$$

which proves the claim. □

The following result is an immediate consequence of Lemma 4.9.15.

Lemma 4.11.4. *Let ϕ be a continuous, positive definite function on G, and let ν be the corresponding measure on the dual group $\widehat{G}$ according to Bochner (Theorem* 4.8.4*). Then, ϕ is transformable as a measure, and its Fourier transform is $\nu^{\dagger}$.* □

Theorem 4.11.5 ([5, Thm. 4.5])**.** *Any positive definite Radon measure μ on G is transformable, and its Fourier transform $\widehat{\mu}$ is positive.*

PROOF. For each $f \in C_{\mathsf{c}}(G)$, the function $\mu * f * \widetilde{f}$ is continuous and positive definite, so, by Theorem 4.8.4 (Bochner), there exists a finite positive measure μ_f such that

$$\mu * f * \widetilde{f} \;=\; \widetilde{\mu_f}.$$

Then, by Lemma 4.11.4, $\mu * f * \widetilde{f}$ is transformable, with μ_f as its Fourier transform.

Observe that, if $f, g \in C_{\mathsf{c}}(G)$, both $\left|\widehat{f}\right|^2 \mu_g$ and $|\widehat{g}|^2 \mu_f$ are the Fourier transforms of the positive definite function $\mu * f * \widetilde{f} * g * \widetilde{g}$, hence

$$\left|\widehat{f}\right|^2 \mu_g \;=\; |\widehat{g}|^2 \mu_f. \tag{4.11.1}$$

Let $h \in C_{\mathsf{c}}(\widehat{G})$. Pick an $f \in C_{\mathsf{c}}(G)$ so that $\widehat{f}(\chi) \neq 0$ for all $\chi \in \operatorname{supp}(h)$. Define the function h_f on $\widehat{G}$ by

$$h_f(\chi) \;=\; \frac{h}{\left|\widehat{f}\right|^2}(\chi) \;:=\; \begin{cases} \frac{h(\chi)}{|\widehat{f}(\chi)|^2}, & \text{if } h(\chi) \neq 0, \\ 0, & \text{if } h(\chi) = 0. \end{cases}$$

We observe from Eq. (4.11.1) that, if $g \in C_{\mathsf{c}}(G)$ is another such function, then

$$\langle \mu_f, h_f \rangle \;=\; \int_G h_f \,\mathrm{d}\mu_f \;=\; \int_G \mathrm{d}(h_f \mu_f) \;=\; \int_G \mathrm{d}(h_g \mu_g) \;=\; \langle \mu_g, h_g \rangle$$

and we can thus unambiguously define a measure σ on G by

$$\langle \sigma, h \rangle \;=\; \langle \mu_f, h_f \rangle.$$

Indeed, it is clear that σ is a positive linear form on $C_{\mathsf{c}}(\widehat{G})$, and thus it is a positive measure; see Remark 4.9.4(i).

Now, let $f \in C_{\mathsf{c}}(G)$ and $h \in C_{\mathsf{c}}(\widehat{G})$ be arbitrary, and let $g \in C_{\mathsf{c}}(G)$ be such that $\widehat{g}(\chi) \neq 0$ for all $\chi \in \operatorname{supp}(h)$. Then,

$$\begin{aligned} \langle \mu_f, h \rangle \;&=\; \big\langle \mu_f, h_g |\widehat{g}|^2 \big\rangle \;=\; \big\langle |\widehat{g}|^2 \mu_f, h_g \big\rangle \;=\; \big\langle |\widehat{f}|^2 \mu_g, h_g \big\rangle \\ &=\; \big\langle \mu_g, (h\,|\widehat{f}|^2)_g \big\rangle \;=\; \big\langle \sigma, h\,|\widehat{f}|^2 \big\rangle \;=\; \big\langle |\widehat{f}|^2 \sigma, h \big\rangle, \end{aligned}$$

showing that $\mu_f = |\widehat{f}|^2 \sigma$ for all $f \in C_{\mathsf{c}}(G)$. Since μ_f is specified by Theorem 4.8.4 (Bochner), we have, for all $f \in C_{\mathsf{c}}(G)$, the following properties:

(i) The measure $\mu_{f^\dagger} = |\widehat{f^\dagger}|^2 \sigma = |\check{f}|^2 \sigma$ is finite, and thus $\check{f} \in L^2(\sigma)$.

(ii) For all $x \in G$,

$$\big(\mu * f^\dagger * \widetilde{f^\dagger}\big)(x) \;= \widetilde{\mu_{f^\dagger}}(x) = \int_{\widehat{G}} \chi(x) \left|\check{f}\right|^2(\chi) \,\mathrm{d}\sigma(\chi).$$

(iii) In particular, by evaluating at 0, we get $\big\langle \mu, f * \widetilde{f} \,\big\rangle = \big\langle \sigma, \left|\check{f}\right|^2 \big\rangle$.

Thus, μ is transformable with σ being its Fourier transform. □

Using this result together with Theorem 4.10.4, we conclude as follows.

Corollary 4.11.6. *Positive definite and translation bounded Radon measures are elements of* $\mathcal{WAP}(G)$. □

Clearly, the attributes 'positive' and 'positive definite' are dual to each other under Fourier transform. Now, we exlore what conclusions can be drawn from measures that are both positive and positive definite.

Theorem 4.11.7. *Let* μ *be a positive and positive definite measure. Then,* μ *is transformable, and* $\widehat{\mu}$ *is a positive and positive definite measure, too.*

Proof. Theorem 4.11.5 gives that μ is transformable and $\widehat{\mu}$ is positive. To prove the positive definiteness of $\widehat{\mu}$, we proceed as follows.

Let $\{g_\alpha\} \subset C_{\mathsf{c}}(G)$ be a non-negative approximate identity for the convolution. For every α, the function

$$f_\alpha \,:=\, \mu * g_\alpha * \widetilde{g_\alpha}$$

is continuous, non-negative and positive definite. Hence, by Lemma 4.9.26, its Fourier transform is

$$\widehat{f_\alpha} \,=\, |\widehat{g_\alpha}|^2 \widehat{\mu}.$$

Since $\widehat{f_\alpha}$ is a finite measure, it is transformable and, by Theorem 4.9.28, its Fourier transform is $f_\alpha^\dagger$, which we already know to be non-negative. Hence, for all $g \in C_{\mathsf{c}}(G)$ and all α, we have

$$\big\langle \widehat{\mu}\, |\widehat{g_\alpha}|^2,\, g * \widetilde{g} \big\rangle \,=\, \big\langle \widehat{f_\alpha}, g * \widetilde{g}\,\big\rangle \,=\, \Big\langle \widehat{\widehat{f_\alpha}}, |\breve{g}|^2 \Big\rangle \,=\, \big\langle f_\alpha^\dagger, |\breve{g}|^2 \big\rangle \,\geqslant\, 0.$$

Since $\{g_\alpha\} \subset C_{\mathsf{c}}(G)$ is an approximate identity, $\lim_\alpha \widehat{g_\alpha} = 1$ holds uniformly on compact subsets of $\widehat{G}$. In particular, for all $g \in C_{\mathsf{c}}(G)$, we have

$$\big\langle \widehat{\mu}, g * \widetilde{g} \big\rangle \,=\, \lim_\alpha \big\langle \widehat{\mu}\, |\widehat{g_\alpha}|^2,\, g * \widetilde{g} \big\rangle \,\geqslant\, 0.$$

Thus, $\widehat{\mu}$ is positive definite. □

Definition 4.11.8. By $\mathcal{M}^+_{\mathsf{pd}}(G)$, we denote the cone of positive and positive definite measures on G.

Corollary 4.11.9. *Any measure* $\mu \in \mathcal{M}^+_{\mathsf{pd}}(G)$ *is Fourier transformable, and its Fourier transform* $\widehat{\mu}$ *is in* $\mathcal{M}^+_{\mathsf{pd}}(\widehat{G})$. □

Lemma 4.11.10. *Let* $\{\mu_\alpha\}$ *be a net of positive definite measures converging, in the vague topology, to a measure* μ*,*

$$\lim_\alpha \mu_\alpha \,=\, \mu.$$

Then, μ *is positive definite and, in the vague topology, we have*

$$\lim_\alpha \widehat{\mu_\alpha} \,=\, \widehat{\mu}.$$

PROOF. We start by proving that μ is positive definite. Indeed, for all functions $f \in C_{\mathsf{c}}(G)$ and all α, we have $\mu_\alpha\bigl(f * \widetilde{f}\bigr) \geqslant 0$. Therefore,

$$\bigl\langle \mu, f * \widetilde{f} \bigr\rangle \,=\, \lim_\alpha \bigl\langle \mu_\alpha, f * \widetilde{f} \bigr\rangle \,\geqslant\, 0.$$

This shows that μ is positive definite.

Next, we show that, for all $f \in C_{\mathsf{c}}(G)$, we have

$$\lim_\alpha |\check{f}\,|^2 \widehat{\mu_\alpha} \,=\, |\check{f}\,|^2 \widehat{\mu}, \tag{4.11.2}$$

in the vague topology.

By the definition of Fourier transformability, we have $\check{f} \in L^2(\widehat{\mu}) \cap L^2(\widehat{\mu_\alpha})$, wherefore the measures $|\check{f}\,|^2\widehat{\mu}$ and $|\check{f}\,|^2\widehat{\mu_\alpha}$ are positive and finite. Furthermore, they are all translation bounded. We can say more: Note that

$$\begin{aligned}\bigl(|\check{f}\,|^2\widehat{\mu}\bigr)(\widehat{G}) \,&=\, \bigl\langle \widehat{\mu}, |\check{f}\,|^2 \bigr\rangle \,=\, \bigl\langle \mu, f * \widetilde{f} \bigr\rangle \,=\, \lim_\alpha \bigl\langle \mu_\alpha, f * \widetilde{f} \bigr\rangle \\ &=\, \lim_\alpha \bigl\langle \widehat{\mu_\alpha}, |\check{f}\,|^2 \bigr\rangle \,=\, \lim_\alpha \bigl(|\check{f}\,|^2\widehat{\mu_\alpha}\bigr)(\widehat{G}).\end{aligned}$$

From this observation, we can conclude that there is an α_0 so that the measures $\{|\check{f}\,|^2\widehat{\mu_\alpha}\}_{\alpha \geqslant \alpha_0}$ are equi-bounded. Using [3, Thm. 2], we see that the set $\{|\check{f}\,|^2\widehat{\mu_\alpha}\}_{\alpha \geqslant \alpha_0}$ is precompact in the vague topology. There is no harm in discarding all indices β in the net which do not satisfy $\alpha_0 \leqslant \beta$, and we shall do this.

To prove that $\lim_\alpha |\widehat{f}\,|^2\widehat{\mu_\alpha} = |\widehat{f}\,|^2\widehat{\mu}$ in the vague topology, it then suffices to show that $|\widehat{f}\,|^2\widehat{\mu}$ is the unique vague cluster point of $\bigl\{|\check{f}\,|^2\widehat{\mu_\alpha}\bigr\}$. Let σ be any cluster point of the net $\bigl\{|\check{f}\,|^2\widehat{\mu_\alpha}\bigr\}$. Then, σ is a finite measure. Moreover, we have

$$\begin{aligned}\bigl\langle |\check{f}\,|^2\widehat{\mu}, \check{h} \bigr\rangle \,&=\, \bigl\langle \widehat{\mu}, |\check{f}\,|^2\check{h} \bigr\rangle \,=\, \bigl\langle \mu, f * \widetilde{f} * h \bigr\rangle \\ &=\, \lim_\alpha \bigl\langle \mu_\alpha, f * \widetilde{f} * h \bigr\rangle \,=\, \lim_\alpha \bigl\langle \widehat{\mu_\alpha}, |\check{f}\,|^2\check{h} \bigr\rangle \,=\, \lim_\alpha \bigl\langle |\check{f}\,|^2\widehat{\mu_\alpha}, \check{h} \bigr\rangle\end{aligned}$$

for all $h \in C_{\mathsf{c}}(G)$.

As σ is a cluster point of $\bigl\{|\check{f}\,|^2\widehat{\mu_\alpha}\bigr\}$ and as the set $\bigl\{\check{h} : h \in C_{\mathsf{c}}(G)\bigr\}$ is dense in $C_0(\widehat{G})$, we see that the finite measure σ is equal to $|\check{f}|^2\widehat{\mu}$ on a dense subset of $C_0(\widehat{G})$, and thus they are equal. This shows Eq. (4.11.2).

Finally, we get rid of the $|\check{f}\,|^2$ as follows. Let $g \in C_{\mathsf{c}}(\widehat{G})$ be arbitrary and let $K = \operatorname{supp}(g)$ and $f \in C_{\mathsf{c}}(G)$ be so that $\check{f} \geqslant 1_K$; see Corollary 4.9.12. Define $h \in C_{\mathsf{c}}(\widehat{G})$ by

$$h(\chi) \,=\, \begin{cases} \frac{g(\chi)}{|\check{f}(\chi)|^2}, & \text{if } \check{f}(\chi) \neq 0, \\ 0, & \text{otherwise.} \end{cases}$$

As $|\check{f}\,|^2\widehat{\mu} = \lim_\alpha |\check{f}\,|^2\widehat{\mu_\alpha}$ in the vague topology, we have

$$\bigl\langle |\check{f}\,|^2\widehat{\mu}, h \bigr\rangle \,=\, \lim_\alpha \bigl\langle |\check{f}\,|^2\widehat{\mu_\alpha}, h \bigr\rangle,$$

and this shows that, for all $g \in C_{\mathsf{c}}(\widehat{G})$, we have

$$\langle \widehat{\mu}, g\rangle \,=\, \lim_{\alpha} \langle \widehat{\mu_\alpha}, g\rangle \,,$$

which proves our claim. □

As a consequence, we get the following result.

Theorem 4.11.11 ([5, Thm. 4.16])**.** *The Fourier transform is a bijection between the cones $\mathcal{M}^+_{\mathsf{pd}}(G)$ and $\mathcal{M}^+_{\mathsf{pd}}(\widehat{G})$. The corresponding inverse mapping $(\check{\cdot})\colon \mathcal{M}^+_{\mathsf{pd}}(\widehat{G}) \longrightarrow \mathcal{M}^+_{\mathsf{pd}}(G)$ is given by*

$$\mu \longmapsto \check{\mu} := \widehat{\mu}^{\dagger}.$$

Moreover, if we equip $\mathcal{M}^+_{\mathsf{pd}}(\widehat{G})$ and $\mathcal{M}^+_{\mathsf{pd}}(G)$ with their vague topologies, the Fourier transform is a homeomorphism. □

The results needed for the theory of diffraction, as we have presented them here, are directed in a way that is somewhat complementary to the aims of [19]. Let us close with three additional results from [19] that the reader may find useful, the last two without proof. Let us begin with a counterpart of Theorem 4.10.4.

Theorem 4.11.12 ([19, Thm. 11.1])**.** *Let μ be a Fourier transformable Radon measure. Then, $\widehat{\mu} \in \mathcal{WAP}(G)$.*

Proof. Let $g \in \mathcal{K}_2(G)$. By Proposition 4.9.25, $\widehat{g}$ and $\widehat{\mu}$ are convolvable as measures and, as an equation in measures, one has

$$\widehat{g} * \widehat{\mu} \,=\, \widehat{g\mu}.$$

As $g\mu$ is a finite measure, $\widehat{g\mu} \in \mathrm{WAP}(G)$. Therefore, using Proposition 4.10.5, $\widehat{g} * \widehat{\mu} = \widehat{g\mu} \in \mathcal{WAP}(G)$. We have thus shown that, for all $g \in \mathcal{K}_2(G)$, one has $\widehat{g} * \widehat{\mu} \in \mathcal{WAP}(G)$.

Now, let $h \in C_{\mathsf{c}}(\widehat{G})$ be fixed. Then, for any function $g \in \mathcal{K}_2(G)$, we have $\widehat{g} * \widehat{\mu} \in \mathcal{WAP}(G)$ and hence $h * \widehat{g} * \widehat{\mu} \in \mathrm{WAP}(G)$. By Theorem 4.9.23, $\widehat{\mu}$ is translation bounded, and hence $h * \widehat{\mu} \in C_{\mathsf{u}}(\widehat{G})$.

Finally, by Proposition 4.9.10, $\widehat{\mathcal{K}_2}(G)$ is dense in $C_0(\widehat{G})$ and thus contains an approximate identity for the convolution algebra $(C_{\mathsf{u}}(\widehat{G}), *)$. Hence, we can find $g_\alpha \in \mathcal{K}_2(G)$ such that

$$h * \widehat{\mu} \,=\, \lim_{\alpha} (h * \widehat{g_\alpha} * \widehat{\mu}) \quad \text{ in } \big(C_{\mathsf{u}}(\widehat{G}), \|.\|_\infty\big).$$

Since $h * \widehat{g_\alpha} * \widehat{\mu} \in \mathrm{WAP}(\widehat{G})$ and $\mathrm{WAP}(\widehat{G})$ is closed in $\big(C_{\mathsf{u}}(\widehat{G}), \|.\|_\infty\big)$, it follows that $h * \widehat{\mu} \in \mathrm{WAP}(\widehat{G})$. □

The modified comparison of Eberlein versus Lebesgue decompositions reads as follows.

Theorem 4.11.13 ([19, Thm. 11.2]). *Let μ be a Fourier transformable Radon measure. Then, μ_{pp} and μ_{c} are Fourier transformable, and one has*

$$\widehat{\mu_{\mathsf{pp}}} = (\widehat{\mu})_{\mathsf{s}} \quad \text{and} \quad \widehat{\mu_{\mathsf{c}}} = (\widehat{\mu})_0 . \qquad \square$$

Corollary 4.11.14 ([19, Cor. 11.1]). *Let $\mu \in \mathcal{M}^\infty(G)$ be Fourier transformable. Then, μ is pure point if and only if $\widehat{\mu} \in \mathcal{SAP}(G)$ and μ is continuous if and only if $\widehat{\mu} \in \mathcal{WAP}_0(G)$.* $\square$

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CHAPTER 5

Almost Periodic Pure Point Measures

Nicolae Strungaru

Motivated by the general structure of mathematical quasicrystals, we construct a cut and project scheme from a family of sets that satisfy some general and fairly natural properties. We use this construction to characterise weighted Dirac combs derived from such a scheme via continuous functions on the internal group in terms of almost periodicity. In particular, we discuss weighted Dirac combs where the internal function is compactly supported. More generally, using the same cut and project construction for ε-dual sets, we characterise Meyer sets in locally compact Abelian groups.[1]

5.1. Introduction

In 1984, D. Shechtman et al. announced the discovery (from 1982) of a solid with an unusual diffraction pattern [42]. While the diffraction was similar to that of a periodic crystal, exhibiting only bright spots (called Bragg peaks) and little or no diffuse background, it also showed fivefold symmetry — a phenomenom which is impossible in a perfect (periodic) crystal in 3-space; see [AO1, Cor. 3.1]. Solids with such unusual (non-crystallographic) symmetries are called (genuine) *quasicrystals*. Such a quasicrystal cannot repeat periodically in a set of directions that span the ambient space. Yet, in order to produce many Bragg peaks, a large number of its local motives (or patches) need to repeat in a highly ordered and coherent fashion.

Twelve years earlier, Y. Meyer [29] introduced the concept of harmonious sets. These sets exhibit long-range order and are usually non-periodic. Meyer also introduced cut and project schemes as a simple way of generating such sets and studied the relationship between harmonious sets and model sets; see below for more on these notions and their connections with the projection method. In the context of icosahedral structures, the latter was independently discovered by P. Kramer and one of his students [19, 21]; see the Epilogue to this volume [20] for a more detailed account and [AO1, Ch. 7] for general

[1]This chapter is dedicated to Robert V. Moody who taught me almost everything I know about Meyer sets.

background. The relevance of Meyer's work to quasicrystals and its relations to the other formulations was realised only in the 1990s; see [30, 22].

Harmonious sets are nowadays also called *Meyer sets*. Their full characterisation by R.V. Moody [30], completing the previous work of Meyer and of Lagarias [22], is surprising in that Meyer sets can be characterised in rather different ways: Via duality, discrete geometry, cut and project schemes, and via the theory of almost lattices. All these different characterisations emphasise that Meyer sets have strong long-range order and that, as was recently shown, this order is manifest in the diffraction pattern as a relatively dense set of Bragg peaks [43] with a high degree of order [44].

A large class of sets that are produced by a cut and project scheme, called the class of *regular* model sets, produce pure point diffraction patterns; see [40, 38] as well as [AO1, Chs. 7 and 9]. Conversely, under suitable additional assumptions, any set with a pure point diffraction pattern can be obtained from a cut and project scheme [6]. Recently, the condition on the regularity of the window was relaxed to a rather natural density assumption on the model set [4, 18]. Here, a *cut and project scheme* (CPS) is a triple $(G, H, \mathcal{L})$ defined by

$$
\begin{array}{ccccc}
G & \xleftarrow{\pi_1} & G\times H & \xrightarrow{\pi_2} & H \\
\cup & & \cup & & \cup \text{ dense} \\
\pi_1(\mathcal{L}) & \xleftarrow{1-1} & \mathcal{L} & \longrightarrow & \pi_2(\mathcal{L}) \\
\| & & & & \| \\
L & & \xrightarrow{\quad\star\quad} & & L^\star
\end{array}
\tag{5.1.1}
$$

with two locally compact Abelian groups G and H and a lattice $\mathcal{L}$ in $G\times H$, subject to the conditions in the diagram; see [30] and [AO1, Ch. 7] for details.

Over the last few years, the connection between cut and project schemes and almost periodic measures has become apparent. Pure point diffraction is equivalent to the *strong* almost periodicity of the autocorrelation measure [12]; see also Corollary 4.10.13 in this volume [33]. However, strong almost periodicity is a concept which often is hard to check. Baake and Moody [7] introduced a stronger concept of almost periodicity, namely *norm*-almost periodicity. For a regular model set, they showed that norm-almost periodicity of the autocorrelation follows from the fact that the covariogram of the window[2] is continuous and compactly supported in the internal space. A nice yet intriguing consequence of this is that the pure point nature of the diffraction spectrum of a regular model set is a result of the continuity of the covariogram. Baake and Moody also showed that, if the autocorrelation of a Meyer

[2]The *covariogram* of a measurable set $W \subseteq G$ is defined as $\mathrm{cvg}_W := 1_W * 1_{-W}$, provided the convolution exists; compare [AO1, Rem. 9.8 and Sec. 9.6.3] for more.

set is norm-almost periodic, there is a natural way of constructing a cut and project scheme from the sets of almost periods of the autocorrelation.

Motivated by some random tiling examples, Richard [37], as well as Lenz and Richard [25], studied a class of weighted Dirac combs (possibly with a dense supporting set) arising from a CPS. More precisely, given a CPS $(G, H, \mathcal{L})$ and a function g on H, we can define a weighted Dirac comb ω_g on G by the diagram

$$\omega_g := \sum_{x \in L} g(x^\star)\, \delta_x .$$

We will often refer to such a measure as a *weighted model comb*.

Since we need the measure ω_g to be translation bounded, g has to be decaying sufficiently fast [37]. Note that, if $g = 1_W$ is the characteristic function of a window W, then ω_g is exactly the Dirac comb of the model set

$$\curlywedge(W) := \{x \in L : x^\star \in W\};$$

compare [AO1, Sec. 7.2]. Moreover, if g is the covariogram of the window, we get exactly the construction of Baake and Moody [7], and, in this case, ω_g is the *autocorrelation* of the model set.

When one studies regular model sets, most of the delicate issues appear around the boundary of the window. Many of these issues seem to come from the fact that ∂W is exactly the set of discontinuities of 1_W. These considerations motivated Lenz and Richard [37, 25] to look at the combs ω_g for continuous functions with fast decay. They showed that, in this case, ω_g is strongly almost periodic [25].

Yet another form of almost periodicity is the *sup*-almost periodicity which appeared in a natural way in the study of the pure point spectrum of a Meyer set [44]. While this concept is more recent than those from [7, 25], looking back to these papers one might also find it hidden in the proof of almost periodicity of the weighted model combs, as a consequence of continuity of the corresponding function on the internal group.

Norm-almost periodicity is the strongest form, implying both strong and sup-almost periodicity. In general, strong and sup-almost periodicity are weaker and are not related to each other. However, for a measure with sparse support, and in particular when the support of the measure is a Meyer set, we will see that the three notions are equivalent. Because of its connection to pure point diffraction, strong almost periodicity is perhaps the most natural concept to study, but we will see below that sup- and norm-almost periodicity are directly related to the cut and project formalism.

The reason why we need sup- or norm-almost periodicity to get the cut and project scheme, and why strong almost periodicity does not seem to work, is interesting and hidden in the construction. Any locally compact

Abelian group (LCAG) G acts by translation on the space of translation bounded measures $\mathcal{M}^\infty(G)$. The group action is continuous in the strong topology, but it is not continuous either in the norm- or in the sup-topology. It is exactly this lack of continuity which allows us to construct the scheme: We will build the CPS from the set of almost periods of an almost periodic measure using the axioms (A1)–(A4) stated in Section 5.2 on page 276 below. While, in general, (A1) and (A3) hold for any (pseudo)-metric and (A4) is equivalent to almost periodicity, we cannot get (A2) unless the group action on $\mathcal{M}^\infty(G)$ fails to be continuous.

The key concepts and results of this chapter are organised as follows. In Section 5.2, we establish that the Baake–Moody construction [7] of a CPS works under weaker assumptions. Given a family of point sets $\{P_\varepsilon\}_{0<\varepsilon<C}$ which satisfies axioms (A1)–(A4) listed at the beginning of the section, and a subgroup L which contains all these sets, we construct a CPS in which the sets $\{P_\varepsilon\}$ are all subsets of model sets. In particular, the Baake–Moody construction works for any pure point sup-almost periodic measure, and we also show that the support function of any such measure defines a uniformly continuous function on the internal group H.

This observation allows us to fully characterise all weighted model combs ω_g given by uniformly continuous functions $g \in C_0(H)$ in terms of sup-almost periodicity as follows.

Theorem 5.4.2. *Let $\varGamma \subseteq G$ be a point set in an LCAG G, and consider a Radon measure $\omega := \sum_{x\in\varGamma} \omega(\{x\})\delta_x$ on G. Then, the following statements are equivalent.*

(i) *The measure ω is sup-almost periodic.*
(ii) *There exists a CPS $(G, H, \mathcal{L})$ and a uniformly continuous window function $g \in C_0(H)$ that vanishes at ∞, such that $\omega = \omega_g$.*

Moreover, the CPS in (ii) *can be chosen such that H is a metrisable group.*

Under the conditions of Theorem 5.4.2, compactness in the internal group can be characterised in terms of the sparseness of the support of the measure. In Section 5.5, we use this to characterise the weighted model (Dirac) combs with $g \in C_{\mathsf{c}}(H)$ in terms of all three types of almost periodicity (Theorem 5.5.2).

The Baake–Moody construction from Section 5.2 also works for the sets of ε-dual characters if these sets are relatively dense, and this permits a characterisation of Meyer sets in any LCAG, similar to the one in [30]. While many of the proofs in [30] are based on the geometry of $\mathbb{R}^d$, and cannot be extended to arbitrary groups G, the strong connection between sup-almost periodicity and cut and project schemes given in Theorem 5.4.2 allows us to

find new proofs for some of these equivalences. Indeed, we are able to prove all of the equivalences except one that was introduced by Lagarias in [22]. However, if G is also compactly generated, we get this last equivalence, too. The main result of Section 5.7 can be summarised as follows.

Theorem 5.7.8. *Let $\varLambda \subseteq G$ be relatively dense, where G is a σ-compact LCAG. Then, the following properties are equivalent.*

(i) *$\varLambda$ is a subset of a model set.*

(ii) *$\varLambda^{\varepsilon}$ is relatively dense for all $0 < \varepsilon < 2$.*

(iii) *$\varLambda^{\varepsilon}$ is a model set for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(iv) *$\varLambda^{\varepsilon}$ is a model set for some $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(v) *$\varLambda^{\varepsilon}$ is relatively dense for some $0 < \varepsilon < \frac{\sqrt{3}}{6}$.*

(vi) *$\varLambda$ is an almost lattice.*

(vii) *$\varLambda - \varLambda - \varLambda$ is locally finite.*

Let us note that, if G is compactly generated, it follows from [6] that property (vii) can be replaced by

(vii') $\varLambda - \varLambda$ is uniformly discrete.

The equivalences in the case of compactly generated LCAGs are summarised in Theorem 5.7.12.

Using this characterisation, we are able to extend all results about the diffraction of Meyer sets from $\mathbb{R}^d$ to an arbitrary LCAG in Section 5.9, and obtain some new characterisations of Meyer sets in terms of almost periods for almost periodic measures.

As already mentioned, Baake and Moody [7] showed that, for a regular model set, both the autocorrelation measure γ and the diffraction measure $\widehat{\gamma}$ can be obtained as weighted model combs. For Meyer sets, we show in Section 5.10 that the same holds for the strongly almost periodic component γ_{s} of the autocorrelation and for the pure point diffraction spectrum $\widehat{\gamma}_{\mathsf{pp}} = \widehat{\gamma_{\mathsf{s}}}$.

5.2. The Baake–Moody construction of a CPS

Note. *Throughout this section, the group G is always assumed to be a locally compact Abelian group (LCAG), which in our setting includes the Hausdorff property.*

The goal of this section is to construct a cut and project scheme (CPS) from a family of subsets $\{P_{\varepsilon}\}$ of G and a subgroup[3] $L \leqslant G$ which satisfy the conditions (A1)–(A5) listed below. It is easy to see that the set of almost

[3]Here and below, we use the symbol $\leqslant$ to denote a subgroup relation.

periods of an almost periodic function verifies conditions (A1), (A3) and (A4). Moreover, if the group action is discontinuous in the topology we consider, condition (A2) usually holds for sufficiently small ε. The requirement (A5) is the only restriction we have on L, and we can easily satisfy this by picking any group L such that $\langle \bigcup_{\varepsilon} P_{\varepsilon} \rangle \leqslant L \leqslant G$. Choosing $L = G$ always works, but sometimes it leads to schemes that are simply too big to be useful. We will see that (A5) is actually not a restriction, but rather a degree of freedom. At the end of this section, we provide some examples to illustrate this point.

Our construction is a variation of the one from [7]. While the latter construction is done for the sets of almost periods P_{ε} of a norm-almost periodic autocorrelation, it only uses certain properties of the sets P_{ε}. In particular, this construction extends to a larger class of almost periodic measures. In Section 5.6, we shall also see a completely different setting in which this basic construction works.

Recall that a set $A \subseteq G$ is called *locally finite* if, for every compact set $K \subseteq G$, the intersection $A \cap K$ is a finite set. This is equivalent to saying that A is closed and discrete in G; see [AO1, Sec. 2.1] for general background on point sets and standard notions used for them.

Given some $C > 0$, a family $\{P_{\varepsilon}\}_{0<\varepsilon<C}$ of subsets of G and a subgroup $L \leqslant G$, our basic requirements (or axioms) are as follows.

(A1) For all $0 < \varepsilon < C$, one has $0 \in P_{\varepsilon}$ as well as $P_{\varepsilon} = -P_{\varepsilon}$.

(A2) For all $0 < \varepsilon < C$, the set P_{ε} is locally finite.

(A3) For all $\varepsilon, \varepsilon'$ with $\varepsilon + \varepsilon' < C$, we have $P_{\varepsilon} + P_{\varepsilon'} \subseteq P_{\varepsilon+\varepsilon'}$.

(A4) For all $0 < \varepsilon < C$, the set P_{ε} is relatively dense.[4]

(A5) For all $0 < \varepsilon < C$, we have $P_{\varepsilon} \subseteq L$.

Before we proceed, let us try to illustrate the idea behind the construction and the meaning of these requirements. Consider a CPS $(G, H, \mathcal{L})$, with H a metrisable LCAG and $\mathcal{L}$ a lattice in $G \times H$, that is, a co-compact discrete subgroup. Define $L := \pi_1(\mathcal{L})$ to be the projection of the lattice $\mathcal{L}$ to G. This is exactly the group L of the CPS (5.1.1).

The star map $\star\colon L \longrightarrow H$ has dense image. We can use this map to induce a topology on L from that of H. Then, H becomes isomorphic to the completion of L with respect to this induced topology. Therefore, if we know $L \leqslant G$ and the correct topology on L, we can recover H. We should also emphasise here that L, with the induced topology, not only gives us H but also the $\star$-map. So, the completion of L with respect to this topology is an LCAG which is isomorphic to H, and the isomorphism takes the inclusion

[4]See footnote on page 176 or [AO1, Sec. 2.1] for the definition of relative denseness.

into the $\star$-map. Moreover, since

$$\mathcal{L} = \big\{(t, t^\star) : t \in L\big\},$$

as soon as we have H and the $\star$-map, we get the lattice $\mathcal{L}$ for free.

Next, let us look at the induced topology on L. As the topology on H is induced by a metric, we can define balls B_ε of radius ε centred at $0 \in H$. The local compactness property of H implies that there exists some $C > 0$ such that B_ε is precompact in H for all $0 < \varepsilon < C$. Since $\{B_\varepsilon\}$ is a fundamental basis of open sets at 0 for the topology of H, we can define a basis of open sets at 0 for the induced topology on L by

$$P_\varepsilon := \star^{-1}(B_\varepsilon) \cap L.$$

Then, $\{P_\varepsilon\}$ is a fundamental basis of open sets at 0 for the induced topology on L. The five conditions (A1)–(A5) are immediate consequences of the choice of $\{B_\varepsilon\}_{0<\varepsilon<C}$ and the fact that $(G, H, \mathcal{L})$ is a CPS.

It is interesting, and perhaps surprising, that the five conditions are not only necessary but also sufficient to produce a CPS. The axioms (A1), (A3) and (A5) are both necessary and sufficient to define a topology on L. Once we take the completion H of L in this topology, we also get a subgroup $\mathcal{L} \subseteq G \times H$. But, in general, the triple $(G, H, \mathcal{L})$ is *not* a CPS. Indeed, axioms (A1), (A3) and (A5) alone are not enough to guarantee that H is an LCAG and, more importantly, that $\mathcal{L}$ is a lattice in $G \times H$.

In the above construction, it is easy to check that the discreteness of $\mathcal{L}$ is equivalent to (A2), which makes this condition both natural and necessary. Moreover, once (A2) is assumed, the relative denseness of $\mathcal{L}$ becomes equivalent to (A4). This makes both conditions (A2) and (A4) necessary for the construction.

We now proceed to the actual construction. Starting with the conditions (A1)–(A5), we step by step define a uniform topology on L, the group H, the $\star$-map, and a lattice $\mathcal{L}$. Then, we prove that we indeed obtain a CPS $(G, H, \mathcal{L})$ this way.

We start by showing that the sets P_ε are decreasing with ε. This is an immediate consequence of (A3) and the fact that $0 \in P_\varepsilon$.

Lemma 5.2.1. *If requirements* (A1) *and* (A3) *hold and* $0 < \varepsilon' < \varepsilon < C$, *one has* $P_{\varepsilon'} \subseteq P_\varepsilon$.

Proof. Let $\varepsilon'' = \varepsilon - \varepsilon' > 0$. By (A1), we have $0 \in P_{\varepsilon''}$, and by (A3), we have $P_{\varepsilon'} + P_{\varepsilon''} \subseteq P_{\varepsilon'+\varepsilon''} = P_\varepsilon$. Thus,

$$P_{\varepsilon'} = P_{\varepsilon'} + 0 \subseteq P_{\varepsilon'} + P_{\varepsilon''} \subseteq P_\varepsilon,$$

which completes the proof. □

The sets P_ε are locally finite by (A2), but this is usually a rather weak requirement. There are many point sets which are locally finite, but which are far from being uniformly discrete.[5] One simple example is

$$\varLambda := \bigl\{ n + \tfrac{k}{n+1} : n \in \mathbb{N} \text{ and } 0 \leqslant k \leqslant n-1 \bigr\}.$$

In the following lemma, we show that, for sufficiently small ε, the sets P_ε are actually uniformly discrete.

Lemma 5.2.2. *If* (A1), (A2) *and* (A3) *hold, one has*

(i) *For all* $0 < \varepsilon < \frac{C}{2}$, *the set* P_ε *has finite local complexity* (*FLC*). *In particular,* P_ε *is uniformly discrete.*

(ii) *For all* $0 < \varepsilon < \frac{C}{4}$, *the set* $P_\varepsilon - P_\varepsilon$ *is uniformly discrete.*

Proof. Combining (A1) and (A3), we get

$$P_\varepsilon - P_\varepsilon \,=\, P_\varepsilon + P_\varepsilon \,\subseteq\, P_{2\varepsilon},$$

provided that $2\varepsilon < C$.

Claim (i). Since $2\varepsilon < C$, the set $P_{2\varepsilon}$ is locally finite by (A2), thus $P_\varepsilon - P_\varepsilon$ is locally finite, which is the FLC property; compare [AO1, Sec. 5.3].

Claim (ii). One has $2\varepsilon < \frac{C}{2}$ and thus, by (i), $P_{2\varepsilon}$ is uniformly discrete. Hence $P_\varepsilon - P_\varepsilon$ is also uniformly discrete. □

If $G = \mathbb{R}^d$ for some d and if the collection $\{P_\varepsilon\}$ satisfies requirements (A1)–(A4), then, combining Lemma 5.2.2 with (A4), we obtain that the sets $\{P_\varepsilon\}_{0<\varepsilon<\frac{C}{4}}$ are Meyer sets. Thus, each of them is a subset of a model set, and embedding some P_ε in a model set, all members of $\{P_{\varepsilon'}\}_{0<\varepsilon'<\varepsilon}$ become, by Lemma 5.2.1, subsets of the same model set. Thus, for some $0 < a < \frac{C}{4}$, the sets $\{P_\varepsilon\}_{0<\varepsilon<a}$ all come from the same CPS.

We shall see later that the same is true under the more general setting of G being a LCAG. Under the assumptions (A1)–(A4), picking any L which satisfies (A5), we will construct a CPS under which all $\{P_\varepsilon\}_{0<\varepsilon<C}$ are subsets of model sets.

Returning to the current construction, we introduce a topology on L for which the family $\{P_\varepsilon\}_{0<\varepsilon<C}$ is a neighbourhood basis of precompact sets. We will need the following lemma, which will imply, later in this section, the precompactness of the P_ε.

Note. *For the remainder of this section, we assume* (A1)–(A5) *to hold in the construction of the CPS.*

---

[5] A subset A of an LCAG G is *uniformly discrete* if there exists an open neighbourhood U of $0 \in G$ such that $(x+U)\cap(y+U) = \varnothing$ holds for all distinct $x, y \in A$. In $\mathbb{R}^d$, this implies the existence of a minimal distance between distinct points; compare [AO1, Sec. 2.1].

Lemma 5.2.3. *Let $0 < \varepsilon' < \varepsilon < C$. Then, there is a finite set F such that*

$$P_\varepsilon \subseteq P_{\varepsilon'} + F.$$

Proof. Since $\varepsilon < C$, there exists $0 < \varepsilon'' < \varepsilon'$ so that $\varepsilon + \varepsilon'' < C$. Then, as $\varepsilon + \varepsilon'' < C$, by (A3) we have

$$P_\varepsilon + P_{\varepsilon''} \subseteq P_{\varepsilon+\varepsilon''}.$$

Now, we use the relative denseness of $P_{\varepsilon''}$ and the fact that $P_{\varepsilon+\varepsilon''}$ is locally finite to find the finite set F. Let $K \subseteq G$ be compact, such that $P_{\varepsilon''} + K = G$. Let $F := K \cap P_{\varepsilon+\varepsilon''}$. Then, by requirement (A2), F is finite. We now show that $P_\varepsilon \subseteq P_{\varepsilon'} + F$.

For all $z \in P_\varepsilon$, there exists $y \in P_{\varepsilon''}$ and $k \in K$ so that $z = y + k$. Then, we get

$$k = z - y \in P_\varepsilon - P_{\varepsilon''} \subseteq P_{\varepsilon+\varepsilon''}.$$

Thus $k \in F$, and since $y \in P_{\varepsilon''} \subseteq P_{\varepsilon'}$, we are done. □

We are now ready to define the topology on L. As it is our goal to make $\{P_\varepsilon\}_{0<\varepsilon<C}$ a neighbourhood basis at 0, the definition of the uniformity $\mathcal{U}$ is straightforward, see [10] for background, and we only need to check that indeed it is a uniformity.

Proposition 5.2.4. *The family $\{P_\varepsilon\}_{0<\varepsilon<C}$ is a neighbourhood basis at 0 for a uniform topology on L.*

Proof. For each $0 < \varepsilon < C$, consider

$$U_\varepsilon := \big\{(x, y) \in L \times L : x - y \in P_\varepsilon\big\}.$$

We show that the set $\mathcal{U} := \big\{U \subseteq L \times L : \exists\, \varepsilon \in (0, C) \text{ so that } U_\varepsilon \subseteq U\big\}$ is a uniformity on L. There are five conditions to be verified.

- **(U1)** $U \in \mathcal{U}, U \subseteq V \subseteq L \times L \implies V \in \mathcal{U}$.
  This is clear from the definition of $\mathcal{U}$.
- **(U2)** $V_1, \ldots, V_n \in \mathcal{U} \implies V_1 \cap V_2 \cap \cdots \cap V_n \in \mathcal{U}$.
  For each $1 \leqslant i \leqslant n$, there exists an $0 < \varepsilon_i < C$ so that $U_{\varepsilon_i} \subseteq V_i$. Let $\varepsilon := \min_{1 \leqslant i \leqslant n}\{\varepsilon_i\}$. Then, $\varepsilon > 0$; $U_\varepsilon \subseteq U_{\varepsilon_i}$ for all $1 \leqslant i \leqslant n$ and hence $U_\varepsilon \subseteq V_1 \cap V_2 \cap \cdots \cap V_n$. Thus, by the definition of $\mathcal{U}$, we have $V_1 \cap V_2 \cap \cdots \cap V_n \in \mathcal{U}$.
- **(U3)** $U \in \mathcal{U} \implies \Delta := \{(x, x) : x \in L\} \subseteq U$.
  This follows from requirement (A1).
- **(U4)** $U \in \mathcal{U} \implies U^{-1} := \{(y, x) : (x, y) \in U\} \in \mathcal{U}$.
  Since $U \in \mathcal{U}$, there exists $0 < \varepsilon < C$ so that $U_\varepsilon \subseteq U$. Then, by requirement (A1), we have $U_\varepsilon \subseteq U^{-1}$.

(U5) $U \in \mathcal{U} \implies \exists V \in \mathcal{U}$ so that[6] $V \circ V \subseteq U$.
This follows from requirement (A3).

This completes the proof. □

Remark 5.2.5. It is easy to see that the family $\{U_\varepsilon\}$ is a fundamental system of entourages for this topology, and one could use this to define the uniformity on L. This shows that $\{P_\varepsilon\}_{0<\varepsilon<C}$ is a neighbourhood basis at 0 for the topology on L.

Moreover, it follows that this topology is metrisable (since $\{P_{\frac{1}{n}}\}_{0<\frac{1}{n}<C}$ is also a neighbourhood basis at 0 for the topology on L). This tells us that the topology on L can also be given by some pseudo-metric. In this case, we can easily define a pseudo-metric by

$$\mathrm{d}(x,y) := \begin{cases} \inf\{\varepsilon : x-y \in P_\varepsilon\}, & \text{if } x-y \in \bigcup_{0<\varepsilon<C} P_\varepsilon, \\ C, & \text{otherwise.} \end{cases}$$

Using requirements (A1) and (A3), it is not difficult to prove that d is indeed a pseudo-metric on L, which yields exactly the same topology as the uniformity from Proposition 5.2.4. ♢

Let H be the completion of $L \neq \{0\}$ in this topology, where here and below we use 'completion' to mean *Hausdorff completion*; see [10] for background. Then, there exists a uniformly continuous map $\phi\colon L \longrightarrow H$ with the following properties.

- **(C1)** The image $\phi(L)$ is dense in H.
- **(C2)** The mapping ϕ is an open mapping from L onto $\phi(L)$, the latter with the induced topology.
- **(C3)** The set $\ker(\phi)$ is the closure of $\{0\} \subset L$ in this topology.

These three properties characterise the pair (H,ϕ) up to isomorphism. Also, note that

$$\ker(\phi) \;=\; \bigcap_{0<\varepsilon<C} P_\varepsilon .$$

Finally, for each $0 < \varepsilon < C$, there exists a neighbourhood $V_\varepsilon \subseteq H$ of 0 such that

$$V_\varepsilon \cap \phi(L) \;=\; \phi(P_\varepsilon).$$

We will frequently make use of this fact; compare [7].

So far, we have constructed the internal group H of our CPS. In order to get a complete CPS, H must be an LCAG. We now show that this is the case. Our proof below is similar to the one of [7, Prop. 1].

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[6]The *composite* of two subsets $U_1, U_2 \subseteq L \times L$ is the set $U_1 \circ U_2$ which is defined as $U_1 \circ U_2 := \{(x,z) : \exists y \in L \text{ with } (x,y) \in U_2 \text{ and } (y,z) \in U_1\}$.

Proposition 5.2.6. *The completion H of L is a metrisable LCAG.*

PROOF. It is clear from the completion process that H is an Abelian group.

We now show that local compactness follows from Lemma 5.2.3. Indeed, P_ε is a precompact set for each $0 < \varepsilon < C$, and hence, by the denseness of $\phi(L)$, the closure $\overline{\phi(P_\varepsilon)} = \overline{V_\varepsilon}$ is a compact neighbourhood of $0 \in H$.

Finally, the metrisability of H follows from Remark 5.2.5, or by observing that $\left\{V_{\frac{1}{n}} : n \in \mathbb{N}\,,\ 0 < \frac{1}{n} < C\right\}$ is a neighbourhood basis at 0 for the topology on H. □

Next, we construct a lattice $\mathcal{L}$ in $G \times H$, which will complete the CPS. As mentioned before, ϕ will be the $\star$-map in this construction, which makes the definition of $\mathcal{L}$ in the following lemma natural.

Lemma 5.2.7. *The set*

$$\mathcal{L} := \left\{(t, \phi(t)) : t \in L\right\}$$

is a lattice in $G \times H$.

PROOF. Since $\mathcal{L}$ is a subgroup of $G \times H$, to prove that it is a lattice we have to show that it is discrete and relatively dense.

Step 1: $\mathcal{L}$ is discrete. The idea for this step is simple: To prove that $\mathcal{L}$ is discrete, it suffices to find an open neighbourhood of 0 in $G \times H$ which intersects $\mathcal{L}$ only at 0. As the topology on $G \times H$ is the product topology, and $\{V_\varepsilon\}$ is a neighbourhood basis at 0 in H, it suffices to find an open set $U \in G$ and some $\varepsilon > 0$ such that $\mathcal{L} \cap (U \times V_\varepsilon) = \{(0, 0)\}$. Any point in this intersection has the form $(t, \phi(t))$ with $t \in U \cap (P_\varepsilon + \ker(\phi))$. Thus, if we can find U and ε such that $U \cap (P_\varepsilon + \ker(\phi)) = \{0\}$, the discreteness of $\mathcal{L}$ follows. As for each $\varepsilon' > \varepsilon$ we have $P_\varepsilon + \ker(\phi) \subseteq P_{\varepsilon'}$, the existence of such a pair follows immediately from requirement (A2).

This reasoning tells us exactly how to prove this result. We start by fixing some $0 < \varepsilon < C$. Next, let us pick some open set $V \subseteq H$ so that $V \cap \phi(L) \subseteq \phi(P_\varepsilon)$. Let $\varepsilon < \varepsilon' < C$. Since $P_{\varepsilon'}$ is locally finite in G, there exists a neighbourhood U of 0 so that $P_{\varepsilon'} \cap U = \{0\}$.

We can now show that $\mathcal{L} \cap (U \times V) = \{(0, 0)\}$. Let $(t, \phi(t)) \in \mathcal{L} \cap (U \times V)$. Then, $t \in L$ and $\phi(t) \in V$, thus $\phi(t) \in V \cap \phi(L) \subseteq \phi(P_\varepsilon)$. Hence, there is some $s \in P_\varepsilon$ with $\phi(s) = \phi(t)$, which implies that $t - s \in \ker(\phi) \subseteq P_{\varepsilon' - \varepsilon}$. This shows that $t = s + (t - s) \in P_\varepsilon + P_{\varepsilon' - \varepsilon} \subseteq P_{\varepsilon'}$. As t is also in U, it follows that

$$t \in P_{\varepsilon'} \cap U \,=\, \{0\},$$

which completes the proof of this step.

Step 2: $\mathcal{L}$ is relatively dense. Let us pick some $0 < \varepsilon < C$. We know that the set $W := \overline{\phi(P_\varepsilon)}$ is compact in H and has non-empty interior. As P_ε is relatively dense in G, there exists a compact set $K \subseteq G$ so that $G = P_\varepsilon + K$.

We now prove that

$$\mathcal{L} + K \times (W - W) = G \times H.$$

Choose some arbitrary $(x, y) \in G \times H$. Since $\phi(L)$ is dense in H, there exists some $z \in L$ so that $y - \phi(z) \in W$. As $G = P_\varepsilon + K$, we can write the difference $x - z$ in the form $x - z = t + k$ with $t \in P_\varepsilon$ and $k \in K$. Thus,

$$\begin{aligned}(x, y) &= (z, \phi(z)) + (x - z, y - \phi(z)) \\ &= (z, \phi(z)) + (t + k, y - \phi(z)) \\ &= (z, \phi(z)) + (t, \phi(t)) + \big(k, [y - \phi(z)] - \phi(t)\big) \\ &\in \mathcal{L} + \mathcal{L} + K \times (W - W) \;=\; \mathcal{L} + K \times (W - W).\end{aligned}$$

Consequently, $(x, y) \in \mathcal{L} + K \times (W - W)$. As the element $(x, y) \in G \times H$ was chosen arbitrarily, it follows that

$$G \times H \;\subseteq\; \mathcal{L} + K \times (W - W),$$

which completes the proof. □

Combining the findings of this section, we obtain the following result.

Theorem 5.2.8. *Let $\big(\{P_\varepsilon\}_{0<\varepsilon<C}, L\big)$ be a pair which satisfies* (A1)–(A5). *Let H be the completion of L in the uniformity for which $\{P_\varepsilon\}_{0<\varepsilon<C}$ is a neighbourhood basis at 0, and let $\phi\colon L \longrightarrow H$ be the corresponding completion map. Define $\mathcal{L} := \big\{(t, \phi(t)) : t \in L\big\}$. Then, H is metrisable and*

$$\begin{array}{ccccc} G & \xleftarrow{\pi_1} & G \times H & \xrightarrow{\pi_2} & H \\ & & \cup & & \\ & & \mathcal{L} & & \end{array} \tag{5.2.1}$$

defines a CPS in the sense of diagram of Eq. (5.1.1), *where $L = \pi_1(\mathcal{L})$ and ϕ is the $\star$-map.* □

We will refer to the construction of the CPS from Theorem 5.2.8 as the *Baake–Moody construction*.

Corollary 5.2.9. *Let $\{P_\varepsilon\}_{0<\varepsilon<C}$ be a collection of sets satisfying conditions* (A1)–(A4). *Then, for all $0 < \varepsilon < C$, the sets*

$$P_\varepsilon + \bigcap_{0<\varepsilon'<C} P_{\varepsilon'}$$

are model sets in the same CPS. In particular, if $\bigcap_{0<\varepsilon'<C} P_{\varepsilon'} = \{0\}$, then, for all $0 < \varepsilon < C$, the sets P_ε are model sets in the same CPS.

PROOF. Consider

$$L := \bigcup_{0<\varepsilon<C} P_\varepsilon .$$

Then, by the Baake–Moody construction, $(G, H, \mathcal{L})$ is a CPS. Also, there exists some precompact set $V_\varepsilon \subseteq H$ with non-empty interior and the property that $\phi(L) \cap V_\varepsilon = \phi(P_\varepsilon)$.

We claim that

$$P_\varepsilon + \bigcap_{0<\varepsilon'<C} P_{\varepsilon'} \,=\, \curlywedge(V_\varepsilon),$$

where $\curlywedge(W) = \{x \in L : x^\star \in W\}$ as before. The inclusion $P_\varepsilon \subseteq \curlywedge(V_\varepsilon)$ follows immediately from $\phi(P_\varepsilon) \subseteq V_\varepsilon$. Moreover, as

$$\bigcap_{0<\varepsilon'<C} P_{\varepsilon'} \,=\, \ker(\phi),$$

we get $P_\varepsilon + \bigcap_{0<\varepsilon'<C} P_{\varepsilon'} \subseteq \curlywedge(V_\varepsilon)$.

To complete the proof, we need to show that $\curlywedge(V_\varepsilon) \subseteq P_\varepsilon + \bigcap_{0<\varepsilon'<C} P_{\varepsilon'}$. Let $x \in \curlywedge(V_\varepsilon)$. Then, $x \in L$ and $\phi(x) \in V_\varepsilon$. This shows that we have $\phi(x) \in \phi(L) \cap V_\varepsilon = \phi(P_\varepsilon)$, and thus $\phi(x) = \phi(y)$ for some $y \in P_\varepsilon$.

Then,

$$x - y \,\in\, \ker(\phi) \,=\, \bigcap_{0<\varepsilon'<C} P_{\varepsilon'},$$

and thus

$$x \,=\, y + (x - y) \,\in\, P_\varepsilon + \bigcap_{0<\varepsilon'<C} P_{\varepsilon'},$$

which completes the proof. □

For a topological group G, we denote the space of uniformly continuous and bounded functions from G to $\mathbb{C}$ by $C_{\mathsf{u}}(G)$. The last question we will address in this section is the following: Given a function $f\colon L \longrightarrow \mathbb{C}$ — when can we lift it through ϕ to some function $g \in C_{\mathsf{u}}(H)$?

As (H, ϕ) is the completion of L, a function f on L can be extended to some $g \in C_{\mathsf{u}}(H)$ if and only if f is bounded and uniformly continuous in the uniformity on L; compare [10, Thm. 3.7.3]. Therefore, we obtain the following simple result.

Lemma 5.2.10. *Let $f\colon L \longrightarrow \mathbb{C}$ be a bounded function with the property that, for each $\varepsilon > 0$, there exists a $\delta > 0$ such that, for all $t \in P_\delta$ and all $x \in L$, we have $|f(t + x) - f(x)| < \varepsilon$. Then, there exists a function $g \in C_{\mathsf{u}}(H)$ such that $f(x) = g(x^\star)$ for all $x \in L$.* □

We complete this section by looking at some explicit examples of the Baake–Moody construction. We start with a simple example which yields $\mathbb{Z}$ as a regular model set. The CPS we get is rather natural, and this example can easily be generalised to treat any lattice in an arbitrary LCAG G.

Example 5.2.11. Let $G = \mathbb{R}$ and $L = \mathbb{Z}$, and let

$$P_\varepsilon \,=\, \mathbb{Z} \quad \text{for any } \varepsilon > 0.$$

In this case, we get $H = \{0\}$ and $\mathcal{L} = \{(n, 0) : n \in \mathbb{Z}\}$. This is the standard CPS that produces $\mathbb{Z}$ as a model set. $\Diamond$

With a minor modification, we can get another CPS which yields $\mathbb{Z}$ with internal group $H = \mathbb{Z}/n\mathbb{Z}$.

Example 5.2.12. Again, set $G = \mathbb{R}$ and $L = \mathbb{Z}$, and let n be a fixed positive integer. Define

$$P_\varepsilon \,=\, n\mathbb{Z} \quad \text{for any } \varepsilon > 0.$$

In this case, we get $H = \mathbb{Z}/n\mathbb{Z}$ and

$$\mathcal{L} \,=\, \bigl\{(m, m \bmod n) : m \in \mathbb{Z}\bigr\} \,\subset\, \mathbb{R}\times(\mathbb{Z}/n\mathbb{Z}),$$

which differs from the previous example. Now, $\mathbb{Z} = \curlywedge(H)$, while one can also describe congruence subsets of $\mathbb{Z}$ modulo n via suitable subsets of H as windows. $\Diamond$

The next example shows what happens when we take advantage of the degree of freedom provided by requirement (A5).

Example 5.2.13. Set $G = \mathbb{R}$ and define again

$$P_\varepsilon \,=\, \mathbb{Z}, \quad \text{for any } \varepsilon > 0.$$

Pick any additive subgroup $L \leqslant \mathbb{R}$ which contains $\mathbb{Z}$. Then, one can check that H is simply the factor group $L/\mathbb{Z}$ equipped with the discrete topology, and that

$$\mathcal{L} \,=\, \bigl\{(\alpha, \alpha + \mathbb{Z}) : \alpha \in L\bigr\} \,\subset\, \mathbb{R}\times(L/\mathbb{Z}).$$

In the particular case when $L = \frac{1}{n}\mathbb{Z}$, we recover Example 5.2.12 up to multiplication by a constant. $\Diamond$

Let us look more closely at an interesting special case of Example 5.2.13. As mentioned before, (A5) is not critical for our construction, and can always be fulfilled by setting $G = L$. But, as we shall see in the next example, this choice typically makes the CPS very big, and it contains redundant information.

Example 5.2.14. Set $G = \mathbb{R}$ and $L = \mathbb{R}$, and define again

$$P_\varepsilon \,=\, \mathbb{Z} \quad \text{for any } \varepsilon > 0.$$

Then, in the Baake–Moody construction, the group H is just the torus

$$\mathbb{R}/\mathbb{Z} \,=:\, \mathbb{T},$$

equipped with the *discrete* topology, that is $H = \mathbb{T}_{\mathsf{d}}$. The lattice $\mathcal{L}$ is

$$\mathcal{L} \,=\, \big\{(\alpha, \alpha \bmod 1) : \alpha \in \mathbb{R}\big\} \,\subset\, \mathbb{R}\times\mathbb{T}_{\mathsf{d}}.$$

We should point out that, in this example, even though our physical group G is simply $\mathbb{R}$, the lattice of the CPS is not countable. Moreover, we have

$$\pi_1(\mathcal{L}) \,=\, \mathbb{R},$$

which looks surprising. The fact that $\mathcal{L}$ is so big does not create any issues, as it is compensated by the sparseness of compact sets in $\mathbb{T}_{\mathsf{d}}$. Indeed, since the compact sets in $\mathbb{T}_{\mathsf{d}}$ are simply the finite sets (due to the discrete topology here), any model set in this scheme is simply a set of the form $\mathbb{Z} + F$, where F is a finite set.

It is not difficult to check that $\mathcal{L}$ is a lattice in $\mathbb{R}\times\mathbb{T}_{\mathsf{d}}$. As the example is a little counterintuitive, we spell out the details.

Discreteness. Let $\lim_n (t_n, t_n+\mathbb{Z}) = (0, 0+\mathbb{Z})$. Then, $\lim_n (t_n+\mathbb{Z}) = 0+\mathbb{Z}$ in $\mathbb{T}_{\mathsf{d}}$, and hence there exists an N so that $t_n + \mathbb{Z} = 0 + \mathbb{Z}$ for all $n > N$. Thus, $t_n \in \mathbb{Z}$ for all $n > N$. Now, since $t_n \in \mathbb{Z}$ and $\lim_n t_n = 0$, there exists some M such that $t_n = 0$ for all $n > M$.

Relative denseness. Let $(x, y + \mathbb{Z}) \in \mathbb{R}\times\mathbb{T}_{\mathsf{d}}$ and let

$$z \,:=\, \lfloor x \rfloor + \langle y \rangle,$$

where $\lfloor . \rfloor$ and $\langle . \rangle$ denote the integer and fractional part of a real number, respectively. Then, $z + \mathbb{Z} = y + \mathbb{Z}$ and $\lfloor x \rfloor = \lfloor z \rfloor$, and we thus find that $x - z \in (-1, 1) \subset [-1, 1]$. Consequently,

$$(x, y+\mathbb{Z}) \,=\, (x, z+\mathbb{Z}) \,=\, (z, z+\mathbb{Z}) + (x-z, 0+\mathbb{Z}) \,\in\, \mathcal{L} + [-1, 1]\times\{0+\mathbb{Z}\},$$

and hence

$$\mathbb{R}\times\mathbb{T}_{\mathsf{d}} \,\subseteq\, \mathcal{L} + [-1, 1]\times\{0+\mathbb{Z}\},$$

which completes the argument. ◊

In the next example, we show that one can use the Baake–Moody construction to create a CPS for $\mathbb{Z}$ with any p-adic group as the internal space.

Example 5.2.15. Let $p \in \mathbb{Z}$ be a prime number. Set $G = \mathbb{R}$ and $L = \mathbb{Z}$. We define P_ε as $P_\varepsilon := P_{\frac{1}{n}} := p^n\mathbb{Z}$ for all $\frac{1}{n+1} < \varepsilon \leqslant \frac{1}{n}$, so that

$$P_\varepsilon \,=\, p^{\lfloor \frac{1}{\varepsilon} \rfloor}\mathbb{Z}.$$

The conditions (A1), (A2), (A4) and (A5) are straightforward to check.

We next see that (A3) also holds. Indeed, it is easy to check that, for all $0 < \varepsilon < \varepsilon'$, we have

$$P_\varepsilon \,\subseteq P_{\varepsilon'}\,.$$

Moreover, as $p^n\mathbb{Z}$ is a subgroup of $\mathbb{Z}$, we have $P_{\varepsilon'} + P_{\varepsilon'} = P_{\varepsilon'}$. Thus, we actually get a *stronger* (non-Archimedean type) version of (A3),

$$P_\varepsilon \,+\, P_{\varepsilon'} \,=\, P_{\max\{\varepsilon,\varepsilon'\}}.$$

It is easy to see that the group H produced by the construction is exactly the group $\mathbb{Z}_p$ of p-adic integers, and that the lattice $\mathcal{L}$ is just the diagonal embedding of $\mathbb{Z}$ in $\mathbb{Z}\times\mathbb{Z}_p \subset \mathbb{R}\times\mathbb{Z}_p$.

A concrete case where this construction can be used (for $p = 2$) is given by the *period doubling* sequence; see [7] and [AO1, Ex. 7.4] for details. ♢

Finally, we use the Baake–Moody construction to rediscover a well-known CPS.

Example 5.2.16. Let α be an irrational number. Set $G = \mathbb{R}^2$ and choose $L = \{a + b\alpha : a, b \in \mathbb{Z}\}$. Then, the sets

$$P_\varepsilon \,:=\, \bigl\{a + b\alpha : a - b\alpha \in (-\varepsilon, \varepsilon)\bigr\},$$

satisfy conditions (A1)–(A5). In this case, it is easy to see that the completion of L in this topology gives $(\mathbb{R}, \phi)$, up to isomorphism, where $\phi\colon\, L \longrightarrow \mathbb{R}$ is defined by

$$\phi(a + b\alpha) \,=\, a - b\alpha.$$

We thus find the expected CPS $(\mathbb{R}, \mathbb{R}, \mathcal{L})$ with the lattice

$$\mathcal{L} \,=\, \bigl\{(a + b\alpha, a - b\alpha) : a, b \in \mathbb{Z}\bigr\} \,=\, \mathbb{Z}\begin{pmatrix}1\\1\end{pmatrix} \oplus \alpha\mathbb{Z}\begin{pmatrix}1\\-1\end{pmatrix}.$$

For $\alpha = \sqrt{2}$, the CPS is exactly the one of the silver mean chain; compare [AO1, Fig. 7.1 and Cor. 7.1]. More generally, one obtains the CPS of one-dimensional model sets that admit an inflation with a quadratic irrationality as its multiplier. Further examples include the Fibonacci chain (with the golden mean) and the noble means chains; compare [AO1, Rem. 4.7 and Ex. 7.3]. ♢

5.3. Almost periodic measures

As detailed in the introduction, the notions of norm-almost periodicity and sup-almost periodicity arise in a natural way in the study of Meyer sets. These concepts are generally much easier to deal with than that of strong almost periodicity. However, the latter is important to the study of mathematical diffraction, as can be seen in Section 4.10. Here, we formally define the two new types of almost periodicity, discuss their basic properties, and establish connections between the different forms of almost periodicity.

On the space of translation bounded measures $\mathcal{M}^\infty(G)$, we employ the norm introduced in [7]; compare Definition 4.9.17. Let $K \subseteq G$ be a fixed compact set with non-empty interior. For a measure $\omega \in \mathcal{M}^\infty(G)$, we define

$$\|\omega\|_K := \sup_{t\in G} |\omega|\,(t+K), \tag{5.3.1}$$

where $|\omega|$ denotes the total variation measure [13]; compare Eq. (4.8.1) as well as [AO1, Sec. 8.5.1] and references therein.

Definition 5.3.1. A translation bounded measure ω is called *norm-almost periodic* if, for all $\varepsilon > 0$, the set[7]

$$P_\varepsilon^K(\omega) := \big\{t \in G : \|\omega - T_t\omega\|_K < \varepsilon\big\}$$

is relatively dense in G. We shall refer to the sets P_ε^K as the *norm-almost periods* of ω.

In line with Definition 4.10.1, ω is called *strongly almost periodic* if, for all functions[8] $f \in C_{\mathsf{c}}(G)$, the function $f * \omega$ is almost periodic.

Remark 5.3.2. If $K' \subseteq G$ is another compact set with non-empty interior, there exist two constants $0 < c \leqslant C < \infty$, so that

$$c\,\|.\|_{K'} \leqslant \|.\|_K \leqslant C\,\|.\|_{K'}.$$

Thus, while different choices of K define different norms, the topology and the concept of norm-almost periodicity are independent of this choice. ♢

As we shall see in Proposition 5.3.3 and in Example 5.3.10 below, norm-almost periodicity is, in general, a stronger requirement than strong almost periodicity.

Proposition 5.3.3 ([7, Lemma 7 and Prop. 8])**.** *Let ω be a translation bounded measure on an LCAG G. Then, the following properties hold.*

(i) *If ω is norm-almost periodic, then ω is strongly almost periodic.*

(ii) *If the set $\operatorname{supp}(\omega) - \operatorname{supp}(\omega)$ is uniformly discrete, then ω is norm-almost periodic if and only if ω is strongly almost periodic.* □

At the end of this section, we shall see that the uniform discreteness condition on the set $\operatorname{supp}(\omega) - \operatorname{supp}(\omega)$ cannot be dropped from statement (ii) of Proposition 5.3.3.

Next, we define a new norm on the space $\mathcal{M}^\infty_{\mathsf{pp}}(G)$ of translation bounded pure point measures by

$$\|\omega\|_\infty := \sup_{x\in G}\big\{|\omega(\{x\})|\big\}.$$

[7] Recall the translation of measures from page 178.

[8] Here and below, $C_{\mathsf{c}}(G)$ denotes the space of continuous $\mathbb{C}$-valued functions with compact support on the group G.

It is easy to see that $\|.\|_\infty$ can also be defined on the space of translation bounded measures. On this space, $\|.\|_\infty$ is a semi-norm, and $\|\mu\|_\infty = 0$ if and only if μ is a continuous measure.

> **Note.** *For the remainder of this chapter, unless stated otherwise, all measures are assumed to be pure point measures. Such a measure, ω say, will often be written as $\omega = \sum_{x\in\varGamma} \omega(\{x\})\,\delta_x$, where the supporting set $\varGamma = \{x \in G : \omega(\{x\}) \neq 0\} \subseteq G$ has an at most countable intersection with any compact set.*

Definition 5.3.4. A pure point measure ω is called *sup-almost periodic* if, for all $\varepsilon > 0$, the set

$$\begin{aligned} P_\varepsilon^\infty(\omega) &:= \Big\{ t \in G : \|\omega - T_t\omega\|_\infty < \varepsilon \Big\} \\ &= \Big\{ t \in G : \sup_{x\in G} \big\{ |\omega(\{t+x\}) - \omega(\{x\})| \big\} < \varepsilon \Big\} \end{aligned}$$

is a relatively dense subset of G. We shall refer to the sets $P_\varepsilon^\infty(\omega)$ as the *sup-almost periods* of ω.

The class of sup-almost periodic measures contains the fully periodic pure point measures, as well as the pure point parts of the diffraction measures of Meyer sets in $\mathbb{R}^d$ [44]. We will see later in this chapter that there is an unexpected yet important connection between sup-almost periodic measures and cut and project schemes.

Next, we study the connection between norm- and sup-almost periodicity. The next two results show that norm-almost periodicity implies sup-almost periodicity, and that, for measures with weakly uniformly discrete[9] support, the two concepts are equivalent.

Lemma 5.3.5. *Let ω be a translation bounded, pure point measure on G and $K \subseteq G$ be a compact set. Then,*

$$\|\omega\|_\infty \leqslant \|\omega\|_K .$$

Proof. Pick some $k \in K$. Since, for any $x \in G$, we have $x = x - k + k \in x - k + K$, we get

$$|\omega(\{x\})| \leqslant |\omega|(x - k + K).$$

Thus, the assertion $\|\omega\|_\infty \leqslant \|\omega\|_K$ is clear. □

[9] A set $\varGamma \subseteq G$ is called *weakly uniformly discrete* if, for each compact $K \subseteq G$ and for all $t \in G$, $\mathrm{card}(\varGamma \cap (t + K))$ is bounded by a constant that depends only on K. This is equivalent to $\delta_\varGamma$ being a translation bounded measure.

Let us point out that translation boundedness is not a necessary condition above. Indeed, if the measure ω fails to be translation bounded, we have $\|\omega\|_K = \infty$, and the inequality of Lemma 5.3.5 is trivially true.

Lemma 5.3.6. *Let $\omega := \sum_{x\in\varGamma} \omega(\{x\})\, \delta_x$ be a translation bounded, pure point measure on G. Then, the following statements are true.*

(i) *If ω is norm-almost periodic, then ω is sup-almost periodic.*

(ii) *If $\varGamma$ is weakly uniformly discrete, then ω is norm-almost periodic if and only if ω is sup-almost periodic.*

Proof. Claim (i) follows immediately from Lemma 5.3.5.

For claim (ii), let $K \subseteq G$ be compact. We know that there exists an $N > 0$ such that, for all $x \in G$, we have $\operatorname{card}(\varGamma \cap (x + K)) \leqslant N$. Let $t \in G$. Then,

$$\begin{aligned}
|T_t\omega - \omega|\,(x+K) &= \sum_{y\in[\varGamma\cup(-t+\varGamma)]\cap(x+K)} |T_t\omega - \omega|\,(\{y\}) \\
&\leqslant \sum_{y\in[\varGamma\cup(-t+\varGamma)]\cap(x+K)} \|T_t\omega - \omega\|_\infty \\
&= \operatorname{card}\big([\varGamma\cup(-t+\varGamma)]\cap(x+K)\big)\, \|T_t\omega - \omega\|_\infty \\
&\leqslant 2N \|T_t\omega - \omega\|_\infty .
\end{aligned}$$

Consequently, we have the norm estimate

$$\|T_t\omega - \omega\|_K \leqslant 2N \|T_t\omega - \omega\|_\infty ,$$

which implies

$$P^\infty_{\frac{\varepsilon}{2N}}(\omega) \subseteq P^K_\varepsilon(\omega).$$

This completes the proof. □

We finish this section by studying the norm- and sup-almost periodicity of a Dirac comb $\delta_\varGamma$. We show that both norm-almost periodicity and sup-almost periodicity are equivalent to $\varGamma$ being a fully periodic (or crystallographic) point set; see [AO1, Sec. 3.1] for background on this concept.

Lemma 5.3.7. *Let $\varGamma \subseteq G$ be a weakly uniformly discrete set, $0 < \varepsilon < 1$ and $t \in G$. Then, the following statements are equivalent.*

(i) $\|T_t(\delta_\varGamma) - \delta_\varGamma\|_K \leqslant \varepsilon$;

(ii) $\|T_t(\delta_\varGamma) - \delta_\varGamma\|_\infty \leqslant \varepsilon$;

(iii) $t + \varGamma = \varGamma$.

Proof. The implications (iii) $\Longrightarrow$ (i) $\Longrightarrow$ (ii) are clear; see Lemma 5.3.6(i). We now prove that (ii) $\Longrightarrow$ (iii).

Let $x \in \varGamma$. Then, we have $|\delta_{\varGamma}(\{-t+x\}) - \delta_{\varGamma}(\{x\})| < \varepsilon$ for any $t \in G$. Thus, we find that

$$|\delta_{\varGamma}(\{-t+x\}) - 1| < 1 \implies \delta_{\varGamma}(\{-t+x\}) \neq 0 \implies x \in t + \varGamma.$$

This proves that $\varGamma \subseteq t + \varGamma$.

The other inclusion is analogous. Let $x \in t + \varGamma$. Then, $x = t + y$ for some $y \in \varGamma$ and, since

$$|\delta_{\varGamma}(\{y\}) - \delta_{\varGamma}(\{t+y\})| \, < \, \varepsilon,$$

we have $|1 - \delta_{\varGamma}(\{x\})| < 1 \Longrightarrow \delta_{\varGamma}(\{x\}) \neq 0 \Longrightarrow x \in \varGamma$. Hence $t + \varGamma \subseteq \varGamma$. □

An immediate consequence of Lemma 5.3.7 is the following result.

Corollary 5.3.8. *Let $\varGamma \subseteq G$ be a weakly uniformly discrete set. Then, the following statements are equivalent.*

(i) *The measure $\delta_{\varGamma}$ is norm-almost periodic.*
(ii) *The measure $\delta_{\varGamma}$ is sup-almost periodic.*
(iii) *$P^{\infty}_{\varepsilon}(\delta_{\varGamma})$ is relatively dense in G for some $0 < \varepsilon < 1$.*
(iv) *$P^{K}_{\varepsilon}(\delta_{\varGamma})$ is relatively dense in G for some $0 < \varepsilon < 1$.*
(v) *The set $\mathrm{per}(\varGamma) := \{t \in G : t + \varGamma = \varGamma\}$ is a lattice.*
(vi) *There exists a lattice L and a finite set F so that $\varGamma = L + F$.* □

In Lemma 5.3.7, weak uniform discreteness is only needed to make sure that norm-almost periodicity makes sense. If $\varGamma$ is not weakly uniformly discrete, the equivalence (ii) $\Longleftrightarrow$ (iii) still holds, and we can prove the following result.

Corollary 5.3.9. *Let $\varGamma \subseteq G$ be a locally finite point set. Then, the following statements are equivalent.*

(i) *The measure $\delta_{\varGamma}$ is sup-almost periodic.*
(ii) *$P^{\infty}_{\varepsilon}(\delta_{\varGamma})$ is relatively dense in G for some $0 < \varepsilon < 1$.*
(iii) *The set $\mathrm{per}(\varGamma) := \{t \in G : t + \varGamma = \varGamma\}$ is a lattice.*
(iv) *There exists a lattice L and a set J such that $\varGamma = L + J$.* □

Note that, for $\varGamma$ as in Corollary 5.3.9, we have the following chain of equivalences: $\delta_{\varGamma}$ is a Radon measure if and only if J (from claim (iv)) is finite, if and only if $\varGamma$ is weakly uniformly discrete, if and only if $\delta_{\varGamma}$ is translation bounded.

We complete this section by providing a simple example of a measure that is strongly almost periodic, but neither norm- nor sup-almost periodic.

Example 5.3.10. Consider the measure

$$\omega \, := \, \delta_{\mathbb{Z}^2} + \delta_{(\mathbb{Z} \times \pi\mathbb{Z}) + (\frac{1}{2}, 0)}.$$

Individually, both measures $\delta_{\mathbb{Z}^2}$ and $\delta_{(\mathbb{Z}\times\pi\mathbb{Z})+(\frac{1}{2},0)}$ are fully periodic, thus also strongly, norm- and sup-almost periodic.

Since the sum of two strongly almost periodic measures is still strongly almost periodic, see Section 4.10.1 or [12], ω is strongly almost periodic. By Corollary 5.3.8, however, ω is neither sup- nor norm-almost periodic. $\Diamond$

As $\mathrm{supp}(\omega)$ is uniformly discrete, the condition (in Proposition 5.3.3) that the set $\mathrm{supp}(\omega) - \mathrm{supp}(\omega)$ is uniformly discrete cannot be weakened to $\mathrm{supp}(\omega)$ being uniformly discrete. Later, after the proof of Theorem 5.5.2, it will become natural to ask whether the above condition can be weakened to finite local complexity of $\mathrm{supp}(\omega)$. The author presently does not know the answer to this question.

5.4. Dense weighted model combs

In this section, we introduce a class of measures that are defined by a CPS together with a continuous function on the internal space. We then study the connection between these measures and sup-almost periodicity.

Definition 5.4.1. Let $(G, H, \mathcal{L})$ be a CPS. We say that $g\colon H \longrightarrow \mathbb{C}$ is a *window function* if the expression

$$\omega_g := \sum_{\ell\in\mathcal{L}} g(\pi_2(\ell))\, \delta_{\pi_1(\ell)} = \sum_{x\in L} g(x^\star)\, \delta_x$$

defines a Radon measure on G, where $L = \pi_1(\mathcal{L})$ according to the CPS diagram of Eq. (5.1.1). In this case, we will call the measure ω_g a *weighted model comb*, and we will refer to g as its *associated function*. If, in addition, $g \in C_{\mathsf{u}}(G)$, we will refer to ω_g as a *continuous weighted model comb*.

Below, we will not address the question of which functions g are window functions; this will always be part of our assumptions.

We now show that any sup-almost periodic pure point Radon measure originates from a CPS. The key for the next theorem is the fact that, given such a measure ω, the family $\{P^\infty_\varepsilon(\omega)\}$ satisfies the requirements (A1)–(A5) of Section 5.2.

Theorem 5.4.2. *Let $\varGamma \subseteq G$ be a point set in an LCAG G, and consider a pure point Radon measure of the form $\omega := \sum_{x\in\varGamma} \omega(\{x\})\delta_x$ on G. Then, the following statements are equivalent.*

(i) *The measure ω is sup-almost periodic.*

(ii) *There exists a CPS $(G, H, \mathcal{L})$ and a uniformly continuous window function $g \in C_0(H)$ such that $\omega = \omega_g$.*

Moreover, the CPS in (ii) *can be chosen such that H is a metrisable group.*

PROOF. To show that (ii) $\Longrightarrow$ (i), we sketch an argument that recently came up in a discussion with Baake, Lenz and Richard. The main idea is that a small translation in H does not change g too much. Therefore, as every open set $U \subseteq H$ yields a relatively dense set $\curlywedge(U)$, it follows that the sets P_ε are relatively dense. We now turn this argument into a formal proof.

Let $\varepsilon > 0$ be arbitrary but fixed. Since g is uniformly continuous, there exists a precompact open set $U \subseteq H$ so that, for all $t \in U$, we have

$$\|g - T_t g\|_\infty < \varepsilon.$$

Then, for all $x \in \pi_1(\mathcal{L})$ and $t \in \curlywedge(U)$, we have

$$|\omega_g(\{x+t\}) - \omega_g(\{x\})| \,=\, |g(x^\star + t^\star) - g(x^\star)| \,<\, \varepsilon.$$

Therefore, $\curlywedge(U) \subseteq P_\varepsilon^\infty(\omega_g)$. Since $\curlywedge(U)$ is relatively dense [30] (compare [AO1, Prop. 7.2]), so is $P_\varepsilon^\infty(\omega_g)$.

To prove the implication (i) $\Longrightarrow$ (ii), we first verify that $\|\omega\|_\infty < \infty$. Let $K' \subseteq G$ be compact with $P_1^\infty(\omega) + K' = G$. Then, it is easy to see that, for all $x \in G$, we have

$$|\omega|(\{x\}) \,\leqslant\, 1 + |\omega|(K') \,<\, \infty.$$

We now claim that the pair $\big(\{P_\varepsilon(\omega)\}_{0<\varepsilon<\|\omega\|_\infty}, L := \langle \varGamma \rangle\big)$ satisfies conditions (A1)–(A5), wherefore the Baake–Moody construction yields our CPS.

Condition (A1) is clear.

Condition (A2) is proved by contradiction. Let $0 < \varepsilon < \|\omega\|_\infty$ and assume that P_ε is not locally finite. Then, there exists a compact set $K' \subseteq G$ such that $\mathrm{card}(P_\varepsilon \cap K') = \infty$. Pick a $y \in \varGamma$ so that $|\omega(\{y\})| > \varepsilon$. Then,

$$|\omega(\{y+t\})| \,>\, |\omega(\{y\})| - \varepsilon \,>\, 0$$

holds for all $t \in P_\varepsilon \cap K'$. Hence,

$$|\omega|(y + K') \,\geqslant \sum_{t \in P_\varepsilon \cap K'} |\omega|(\{y+t\}) \,\geqslant\, \big(|\omega(\{y\})| - \varepsilon\big)\, \mathrm{card}(P_\varepsilon \cap K') \,=\, \infty.$$

But this contradicts the regularity of ω, so P_ε must be locally finite.

Condition (A3) follows from the triangle inequality.

Condition (A4) is equivalent to ω being sup-almost periodic.

Finally, consider condition (A5). Let $0 < \varepsilon < \|\omega\|_\infty$ and choose $x \in \varGamma$ so that $\varepsilon < |\omega(\{x\})|$. Then, for each $t \in P_\varepsilon$, we have

$$|\omega(\{x+t\})| \,\geqslant\, |\omega(\{x\})| - \varepsilon \,>\, 0.$$

Thus $t + x \in \varGamma$, so $t \in -x + \varGamma$. We conclude that

$$P_\varepsilon \,\subseteq\, -x + \varGamma \,\subseteq\, \varGamma - \varGamma \,\subseteq\, L.$$

Hence, the pair $\big(\{P_\varepsilon(\omega)\}_{0<\varepsilon<\|\omega\|_\infty}, L := \langle \varGamma \rangle\big)$ satisfies conditions (A1)–(A5). By Theorem 5.2.8, we now get a CPS $(G, H, \mathcal{L})$ with H metrisable.

Let $f\colon L \longrightarrow \mathbb{C}$ be defined by $f(x) = \omega(\{x\})$. Then, one has

$$f(x) \,=\, \begin{cases} \omega(\{x\}), & \text{for } x \in \varGamma, \\ 0, & \text{otherwise.} \end{cases}$$

Let $t \in P_\varepsilon$ and $x \in L$. Since $t + x \in L$, we get

$$|f(t+x) - f(x)| \,=\, |\omega(\{t+x\}) - \omega(\{x\})| \,<\, \varepsilon.$$

This shows that f is uniformly continuous in the topology induced on L. Therefore, by Lemma 5.2.10, there exists a function $g \in C_{\mathsf{u}}(H)$ so that

$$f \,=\, g \circ \phi,$$

with the completion map ϕ from above. Then,

$$\omega \,=\, \sum_{x\in L} \omega(\{x\})\, \delta_x \,=\, \sum_{x\in L} f(x)\, \delta_x \,=\, \sum_{x\in L} g(\phi(x))\, \delta_x \,=\, \sum_{x\in L} g(x^\star)\, \delta_x \,=\, \omega_g.$$

The only thing left to prove is that g vanishes at infinity. We will see that this is a consequence of the regularity of the measure.

Firstly, observe that, since ω is a Radon measure, the set

$$S_\varepsilon \,:=\, \big\{x \in G : |\omega(\{x\})| > \varepsilon\big\}$$

is locally finite for all $\varepsilon > 0$. Fix some $\varepsilon > 0$, and let $K' \subseteq G$ be some compact set such that

$$P_{\varepsilon/2} + K' = G.$$

Define $F := S_{\varepsilon/2} \cap K'$. Then, F is a finite subset of L.

Let $W := \{y \in H : |g(y)| > \varepsilon\}$. To complete the proof, we show that W is a subset of the compact set $\overline{\phi(P_{\varepsilon/2}) + \phi(F)}$. Let $y \in W \cap \pi_2(\mathcal{L})$. Then, there exists $x \in S_\varepsilon$ so that $y = \phi(x)$. We can write $x = z + k$ with $z \in P_{\varepsilon/2}$ and $k \in K'$. Then,

$$|\omega(\{k\})| \,=\, |\omega(\{x - z\})| \,\geqslant\, |\omega(\{x\})| - \frac{\varepsilon}{2} \,>\, \frac{\varepsilon}{2}.$$

Thus, $k \in S_{\varepsilon/2} \cap K' = F$. So $x \in P_{\varepsilon/2} + F$, and hence $y \in \phi(P_{\varepsilon/2}) + \phi(F)$.

We have shown that

$$W \cap \pi_2(\mathcal{L}) \,\subseteq\, \phi(P_{\varepsilon/2}) + \phi(F). \tag{5.4.1}$$

Since $\pi_2(\mathcal{L})$ is dense in H and since W is open, taking the closure on both sides of Eq. (5.4.1) gives

$$W \,\subseteq\, \overline{W \cap \pi_2(\mathcal{L})} \,\subseteq\, \overline{\phi(P_{\varepsilon/2}) + \phi(F)}.$$

Now, we conclude that $|g(y)| \leqslant \varepsilon$ outside the compact set $\overline{\phi(P_{\varepsilon/2}) + \phi(F)}$, which completes the proof. □

Remark 5.4.3.

(i) It is easy to check that, under the conditions of Theorem 5.4.2, we have

$$\bigcap_{\varepsilon'>0} P^{\infty}_{\varepsilon'}(\omega) \,=\, \{t \in G : T_t\omega = \omega\} \,=\, \mathrm{per}(\omega).$$

Therefore, for all $\varepsilon > 0$, we have

$$P^{\infty}_{\varepsilon}(\omega) + \bigcap_{\varepsilon'>0} P^{\infty}_{\varepsilon'}(\omega) \,=\, P^{\infty}_{\varepsilon}(\omega).$$

(ii) The fact that ω is a Radon measure is essential for the discreteness of the P_ε and thus the construction of the CPS. Note that, for instance, the formal sum $\delta_{\mathbb{Q}}$ is sup-almost periodic in $\mathbb{R}$, but not a measure, and the set of almost periods does not produce a CPS.

(iii) The condition that $g \in C_0(H)$ is a necessary but not a sufficient condition for ω to be a Radon measure.

(iv) Under the conditions of Theorem 5.4.2, the denseness of $L^\star$ in H implies that

$$P^{\infty}_{\varepsilon}(\omega_g) \,=\, \{t \in L : \|T_{t^\star} g - g\|_\infty \leqslant \varepsilon\}.$$

It is easy to conclude that the topology on H is given by the metric

$$\mathrm{d}(h, k) = \|T_h g - T_k g\|_\infty.$$

This explains why the topology on H is metrisable. ◊

Combining Theorem 5.4.2, Corollary 5.2.9 and Remark 5.4.3(i), we obtain the following result.

Corollary 5.4.4. *Let ω be a pure point Radon measure on G. If, in addition, ω is sup-almost periodic, then, for all $0 < \varepsilon < \|\omega\|_\infty$, the sets $P^{\infty}_{\varepsilon}(\omega)$ are model sets in the same CPS.* □

In the same way as above, we can prove the following result.

Lemma 5.4.5. *Let ω be a translation bounded, pure point measure on G. If ω is norm-almost periodic with respect to $\|.\|_K$, there exists a $C > 0$ such that the sets $P^{K}_{\varepsilon}(\omega)$ with $0 < \varepsilon < C$ are model sets in the same CPS.*

Proof. We show that $\{P^{K}_{\varepsilon}(\omega)\}_{0<\varepsilon<\|\omega\|_\infty}$ satisfies (A1)–(A4), and thus, by Corollary 5.2.9, the sets $P^{K}_{\varepsilon}(\omega)$ are all model sets.

Conditions (A1) and (A3) are obvious, while (A4) is equivalent to norm-almost periodicity.

Since ω is norm-almost periodic, it is sup-almost periodic, and we showed in Theorem 5.4.2 that, for all $0 < \varepsilon < \|\omega\|_\infty$, the set $P^{\infty}_{\varepsilon}(\omega)$ is locally finite. Since $P^{K}_{\varepsilon}(\omega) \subseteq P^{\infty}_{\varepsilon}(\omega)$, condition (A2) also holds. □

Note that Lemma 5.4.5 is not necessarily true for measures with a continuous component. The following lemma shows that, if $f \in C_{\mathsf{u}}(G)$ is an almost periodic function in the sense of Bohr (compare Section 4.1.1 or [AO1, Sec. 8.2]), the measure[10] $\mu = f\theta_G$ is a norm-almost periodic measure. Note that, in this case, the set of norm-almost periods of μ need not be locally finite.

Lemma 5.4.6. *Let $f \in C_{\mathsf{u}}(G)$ and consider $\omega = f\theta_G$. Then, ω is norm-almost periodic if and only if f is a Bohr-almost periodic function.*

Proof. Direction $\Longrightarrow$ is immediate: Since $f\theta_G$ is a norm-almost periodic measure, by Proposition 5.3.3 it is a strongly almost periodic measure as well. As $f \in C_{\mathsf{u}}(G)$, it follows from Proposition 4.10.5 that f is an almost periodic function.

To show $\Longleftarrow$, let K be a compact set with non-empty interior. Now, if t is an ε-almost period of f, we have $\|f - T_t f\|_\infty < \varepsilon$. Therefore, one gets

$$\begin{aligned} \|\omega - T_t\omega\|_K &= \sup_{x\in G} \bigl|\omega - T_t\omega\bigr|(x+K) \\ &= \sup_{x\in G} \int_{x+K} |f(y) - f(-t+y)| \,\mathrm{d}\theta_G(y) \\ &\leqslant \sup_{x\in G} \int_{x+K} \varepsilon \,\mathrm{d}\theta_G(y) \;=\; \varepsilon\, \theta_G(K). \end{aligned}$$

Therefore, every ε-almost period of f is an $\bigl(\varepsilon\theta_G(K)\bigr)$-norm almost period of ω. As $\theta_G(K)$ is a fixed constant, which does not depend on ε, the desired conclusion follows. □

5.5. Continuous weighted model combs

In this section, we characterise weighted model combs associated with a continuous function of compact support.

The next lemma will be an important tool for many of the results to come. In the particular case $G = \mathbb{R}^d$, this result was proved in [43, Lemma 3.10], and essentially the same proof works in the case of a general LCAG. We include the proof below for completeness.

Lemma 5.5.1. *Let $B \subseteq A \subseteq G$. If B is relatively dense in G and if A has finite local complexity, then there exists a finite set F such that $A \subseteq B + F$.*

Proof. Let $K \subseteq G$ be a compact set such that $B + K = G$. Now, define $F := K \cap (A - A)$, which is a finite set because $A - A$ is discrete and closed.

[10] Here and below, θ_G denotes the standard Haar measure of the LCAG G.

We now show that $A \subseteq B+F$. Let $x \in A$. Then, $x \in B+K$, so $x = y+k$ with $y \in B$ and $k \in K$. Consequently, $k = x - y \in (A-B) \cap K \subseteq F$. Since $x = y + k$ with $y \in B$ and $k \in F$, we are done. □

In the previous section, we proved that any sup-almost periodic pure point measure comes from a CPS in conjunction with a uniformly continuous function. We can now use Lemma 5.5.1 to show that, if such a measure is supported on a set of finite local complexity, the associated function g on H is compactly supported, and the CPS $(G, H, \mathcal{L})$ can be chosen such that H is compactly generated and metrisable. Thus, we obtain the following result.

Theorem 5.5.2. *Let $\omega = \sum_{x \in \varGamma} \omega(\{x\})\, \delta_x$ be a translation bounded Radon measure, with supporting set $\varGamma$. Then, the following statements are equivalent,*

(i) *ω is norm-almost periodic and $\varGamma$ has finite local complexity;*
(ii) *ω is norm-almost periodic and $\varGamma - \varGamma$ is uniformly discrete;*
(iii) *ω is strongly almost periodic and $\varGamma - \varGamma$ is uniformly discrete;*
(iv) *ω is sup-almost periodic and $\varGamma - \varGamma$ is uniformly discrete;*
(v) *ω is sup-almost periodic and $\varGamma$ has finite local complexity;*
(vi) *there exists a CPS $(G, H, \mathcal{L})$ and a function $f \in C_{\mathsf{c}}(H)$ so that*

$$\omega \,=\, \omega_f \,=\, \sum_{x \in L} f(x^{\star})\, \delta_x .$$

Moreover, the CPS in (vi) *can be chosen such that H is a compactly generated metrisable group.*

Proof. The equivalence (ii) $\iff$ (iii) follows from Proposition 5.3.3, while (ii) $\iff$ (iv) follows from Lemma 5.3.6.

The implication (ii) $\implies$ (i) is obvious, while (i) $\iff$ (v) also follows from Lemma 5.3.6. To complete the proof, we show (v) $\implies$ (vi) $\implies$ (iv).

The implication (vi) $\implies$ (iv) is immediate. The measure ω is translation bounded, thus Radon, and applying Theorem 5.4.2 we get that $\omega = \omega_f$ is sup-almost periodic.

Let W be a compact set in H so that $\mathrm{supp}(f) \subseteq W$. Then, because $\omega(\{x\}) \neq 0$ holds for all $x \in \varGamma$, we have $\varGamma \subseteq \curlywedge(W)$ and $\varGamma - \varGamma \subseteq \curlywedge(W-W)$. Since $W-W$ is compact, it follows that $\varGamma - \varGamma$ is uniformly discrete.

We now prove that (v) $\implies$ (vi). By Theorem 5.4.2, there exists a CPS $(G, H, \mathcal{L})$, with H metrisable, and a function $f \in C_0(H)$ so that $\omega = \omega_f$. We will now show that f is compactly supported.

If $f \equiv 0$, we are done. Otherwise, select some $0 < \varepsilon < \|f\|_{\infty}$. Since $f \in C_0(H)$, the set

$$U \,:=\, \big\{ y \in H : |f(y)| > \varepsilon \big\}$$

is open, non-empty and precompact. Thus, the set $\curlywedge(U)$ is relatively dense, and it is contained in Γ.

Since Γ has finite local complexity, Lemma 5.5.1 implies the existence of a finite set F so that

$$\Gamma \subseteq \curlywedge(U) + F.$$

Moreover, since both $\curlywedge(U)$ and Γ are contained in the group $L = \pi_1(\mathcal{L})$, we can choose F so that $F \subseteq L$ and $F^\star = \{x^\star : x \in F\}$ is well defined.

Define the set

$$V := \{y \in H : f(y) \neq 0\}.$$

We need to show that V is precompact. Since $\pi_2(\mathcal{L})$ is dense in H and V is open, it is sufficient to show that $\overline{\pi_2(\mathcal{L}) \cap V}$ is compact.

Let $y^\star \in \pi_2(\mathcal{L}) \cap V$. Then, there exists a $y \in L$ such that $(y, y^\star) \in \mathcal{L}$. By the very definition of ω, we have $\omega(\{y\}) = f(y^\star) \neq 0$. Hence, we obtain $y \in \Gamma \subseteq \curlywedge(U) + F$, so $y^\star \in U + F^\star$. This shows that $\pi_2(\mathcal{L}) \cap V \subseteq U + F^\star$, and therefore

$$\operatorname{supp}(f) = \overline{\pi_2(\mathcal{L}) \cap V} \subseteq \overline{U} + F^\star,$$

which is compact since U is precompact and $F^\star$ is finite.

Finally, since we chose $L = \langle \Gamma \rangle$ in the Baake–Moody construction in the proof of Theorem 5.4.2, it follows that the group $\pi_2(\mathcal{L}) = L^\star$ is generated by $\Gamma^\star$. Now, pick W to be any compact set with non-empty interior which contains $\operatorname{supp}(f)$. Then, we have $\Gamma^\star \subseteq W$. It follows that the group generated by W is open, hence closed in H, and contains $\pi_2(\mathcal{L})$. This shows that H is generated by W. □

We complete this section by looking at an example that emphasises why we need the freedom of choice of L in requirement (A5).

Example 5.5.3. Let

$$\omega := \delta_{\mathbb{Z}} - \frac{1}{2}\,\delta_{\pi+\mathbb{Z}}.$$

In this case, $C = C(\omega) = 1$ and

$$P_\varepsilon(\omega) = \mathbb{Z}$$

for any $0 < \varepsilon < 1$.

First choice. Let us choose $L = \big\langle \bigcup_{0<\varepsilon<C} P_\varepsilon \big\rangle$, the *smallest* possibility for L. Then, the CPS simply is $\big(\mathbb{R}, \{0\}, \mathbb{Z}\times\{0\}\big)$.

While we get a CPS, ω does not originate from a continuous function $g \in C_{\mathsf{u}}(H)$, though it is a linear combination of translates of such weighted combs (one can show that this is always the case for this choice).

Second choice. Let us choose $L = G$, the *largest* possibility for L. Then, $H = \mathbb{R}/\mathbb{Z}$ is equipped with the discrete topology, and

$$\mathcal{L} = \{(t, t + \mathbb{Z}) : t \in \mathbb{R}\}.$$

Let $g\colon \mathbb{R}/\mathbb{Z} \longrightarrow \mathbb{C}$ be defined by

$$g(0+\mathbb{Z}) \,=\, 1, \quad g(\pi+\mathbb{Z}) \,=\, -\frac{1}{2} \quad \text{and} \quad g(x+\mathbb{Z}) = 0 \text{ otherwise.}$$

This implies $g \in C_{\mathsf{c}}(H)$ and $\omega = \omega_g$.

While this choice of G always works, let us observe that our CPS now is too big: H is an uncountable discrete group, and we only use two of its elements. It should be sufficient to replace H by the subgroup generated by these two elements.

Third choice. Let us choose $L = \langle \mathbb{Z} \cup (\pi+\mathbb{Z}) \rangle$, the group generated by the support of ω. Then, $L = \mathbb{Z} + \pi\mathbb{Z}$ and $H = \pi\mathbb{Z}$, a free Abelian group with one generator. Again, H is equipped with the discrete topology, and

$$\mathcal{L} \,=\, \{(a+b\pi, b\pi) : a, b \in \mathbb{Z}\}.$$

Let $g\colon \pi\mathbb{Z} \longrightarrow \mathbb{C}$ be defined by

$$g(0) \,=\, 1, \quad g(\pi) \,=\, -\frac{1}{2} \quad \text{and} \quad g(x) \,=\, 0 \text{ otherwise.}$$

Then, $g \in C_{\mathsf{c}}(H)$ and $\omega = \omega_g$. ♢

5.6. On ε-dual characters

In this section, we will consider a completely different situation in which the Baake–Moody construction can be used. Starting with a Delone set $\varLambda$ and considering the sets of characters which are almost 1 on $\varLambda$, we obtain a family of sets which satisfy requirements (A1)–(A3). Therefore, as long as (A4) also holds for these sets, we can employ the construction to create a CPS. With this approach, we can extend the characterisation of Meyer sets from $\mathbb{R}^d$ to an arbitrary LCAG.

For a review of the definition and properties of characters and dual groups, as well as Pontryagin duality, we refer the reader to Section 4.2.1 in this volume. Let us begin by defining the sets of characters which are approximately 1 on $\varLambda$.

Definition 5.6.1. Let $\varLambda \subseteq G$ be a relatively dense set. For $\varepsilon > 0$,

$$\varLambda^{\varepsilon} \,:=\, \bigl\{\chi \in \widehat{G} : |\chi(x) - 1| \leqslant \varepsilon \text{ for all } x \in \varLambda\bigr\}$$

is the set of *ε-dual characters* of $\varLambda$.

Remark 5.6.2. It is rather common to use the multiplicative notation for the dual group $\widehat{G}$. However, we will often deal with sets of the form $\varLambda^{\varepsilon} - \varLambda^{\varepsilon}$, which would become $\varLambda^{\varepsilon} \cdot (\varLambda^{\varepsilon})^{-1}$ in multiplicative notation and then look rather confusing. Therefore, we prefer additive notation for characters, but

will distinguish it from the usual addition in G. Thus, for $\chi, \psi \in \widehat{G}$, the sum $\chi \mathbin{\hat{+}} \psi$ is defined by

$$(\chi \mathbin{\hat{+}} \psi)(x) := \chi(x)\,\psi(x) \quad \text{for all } x \in G,$$

where the right-hand side means multiplication of the complex numbers $\chi(x)$ and $\psi(x)$. Likewise, the inverse $\hat{-}\chi$ of a character χ is given by

$$(\hat{-}\chi)(x) := \overline{\chi(x)}.$$

We should note that, with this notation, we have

$$\bigl(-\varLambda\bigr)^{\varepsilon} \,=\, \varLambda^{\varepsilon} \,=\, \hat{-}\bigl(\varLambda^{\varepsilon}\bigr),$$

as can be checked from the definitions. $\Diamond$

Let us now study the ε-dual sets of a Delone set $\varLambda \subseteq G$, where G is an arbitrary LCAG. We will show that, if all the ε-dual sets with $0 < \varepsilon < 2$ are relatively dense, axioms (A1)–(A4) hold, and the Baake–Moody construction yields a CPS in which all $\varLambda^{\varepsilon}$ are model sets. This way, we will be able to prove that most of the equivalent characterisations of Meyer sets in $\mathbb{R}^d$ are still equivalent when formulated in the more general context of LCAGs.

It may look surprising that the theory we built at the beginning of this chapter, with the model of almost periods of sup-almost periodic measures in mind, can also be applied to the ε-dual sets, but there is a simple reason why this happens. Let us explain this a little further.

For a point set $\varLambda$, we denote $\varDelta := \varLambda - \varLambda$. It is easy to see (compare for instance Lemma 5.6.9) that

$$\varLambda^{\varepsilon} \,\subseteq\, \varDelta^{2\varepsilon}.$$

Moreover, as we will see in Section 5.9, there exists a constant $C > 0$ so that the sets $\varDelta^{\varepsilon}$ are $(C\varepsilon)$-almost periods of the pure point diffraction measure $(\widehat{\gamma})_{\mathsf{pp}}$ of $\varLambda$. Thus, if $\varLambda^{\varepsilon}$ is relatively dense for each $\varepsilon > 0$, then $(\widehat{\gamma})_{\mathsf{pp}}$ is sup-almost periodic, and the sets $\varLambda^{\varepsilon}$ are subsets of the model sets given by the ε-sup-almost periods of the measure.

Given $\varLambda \subseteq G$ and its ε-dual $\varLambda^{\varepsilon} \subseteq \widehat{G}$, one can go further and consider the ε-dual of $\varLambda^{\varepsilon}$, that is, $(\varLambda^{\varepsilon})^{\varepsilon} \subseteq \widehat{\widehat{G}} \simeq G$; compare Theorem 4.2.3 on page 182. One then obtains the important relation

$$\varLambda \,\subseteq\, (\varLambda^{\varepsilon})^{\varepsilon}, \tag{5.6.1}$$

which follows from the observation that, if $x \in \varLambda$, we have

$$|x(\chi) - 1| \,=\, |\chi(x) - 1| \,\leqslant\, \varepsilon,$$

for all $\chi \in \varLambda^{\varepsilon}$.

In this section, we will often use iterated ε-duals and their properties. The standard notation $\varLambda^{\varepsilon\varepsilon'}$ [29, 30] for iterated duals can be misleading: $\varLambda^{\varepsilon\varepsilon'}$ can be understood either as the ε'-dual of $\varLambda^{\varepsilon}$, or as the $(\varepsilon\varepsilon')$-dual of $\varLambda$.

Usually, the meaning is clear from the context, as the former is a set in the group G while the latter is a set in $\widehat{G}$, but to avoid any potential issues we will always use brackets for iterated duals, and denote the iterated ε'-dual of $\varLambda^{\varepsilon}$ by $(\varLambda^{\varepsilon})^{\varepsilon'}$. It follows immediately from the definition of $(\varLambda^{\varepsilon})^{\varepsilon'}$ that this operation is associative.

Finally, it is easy to see from the definition that taking ε-duals reverses inclusions as follows.

Fact 5.6.3. *If $\varLambda \subseteq \varGamma$ and $\varepsilon > 0$, one has $\varGamma^{\varepsilon} \subseteq \varLambda^{\varepsilon}$.* □

In particular, by combining this property with Eq. (5.6.1), we find that, for all $\varLambda \subseteq G$ and all $\varepsilon > 0$, we have

$$\bigl((\varLambda^{\varepsilon})^{\varepsilon}\bigr)^{\varepsilon} \,=\, \varLambda^{\varepsilon}.$$

In the first part of this section, we will show that, for a relatively dense set $\varLambda \subseteq G$, the family $\{\varLambda^{\varepsilon}\}_{0<\varepsilon<\sqrt{3}/2}$ satisfies the axioms (A1)–(A3) from page 276. Both (A1) and (A3) are immediate consequences of the definition of $\varLambda^{\varepsilon}$, and even hold if $\varLambda$ is not relatively dense, while (A2) follows from the relative denseness of $\varLambda$.

Lemma 5.6.4. *Let $\varLambda \subseteq G$. Then, the family $\{\varLambda^{\varepsilon}\}_{0<\varepsilon<2}$ satisfies* (A1) *and* (A3) *in $\widehat{G}$.*

Proof. Property (A1) is obvious.

To verify (A3), let $\varepsilon, \varepsilon' > 0$ and let $\chi \in \varLambda^{\varepsilon}$, $\psi \in \varLambda^{\varepsilon'}$. Then, for all $x \in \varLambda$, we have

$$\begin{aligned} |(\chi \mathbin{\hat{+}} \psi)(x) - 1| \,&=\, |\chi(x)\psi(x) - 1| \,=\, |\chi(x)\psi(x) - \chi(x) + \chi(x) - 1| \\ &\leqslant\, |\chi(x)\psi(x) - \chi(x)| + |\chi(x) - 1| \,\leqslant\, \varepsilon + \varepsilon', \end{aligned}$$

completing the proof. □

To prove (A2), we first need a simple lemma, which is a fairly standard result in character theory. Here, we use $\mathbb{C}^* = \mathbb{C} \setminus \{0\}$ for the multiplicative group of complex numbers.

Lemma 5.6.5. *Let H be a subgroup of $\mathbb{S}^1 \subset \mathbb{C}^*$. If $H \neq \{1\}$, there exists some $z \in H$ with $|z - 1| \geqslant \sqrt{3}$.*

Moreover, unless H consists exactly of the third roots of unity, we can find some $z \in H$ such that the inequality is strict.

Proof. Since $H \neq \{1\}$, we can find a $\zeta \in H$ with $\zeta \neq 1$. We have to consider three cases.

First case: $\mathrm{ord}(\zeta) = \infty$, which means that ζ cannot be a root of unity. Then, by an application of Dirichlet's approximation theorem [29, Thm. 1], ζ generates a subgroup which is dense in $\mathbb{S}^1$, and the claim is obvious.

Second case: $\mathrm{ord}(\zeta) = 2n$ for some $n \in \mathbb{N}$. Then, $-1 = \zeta^n \in H$, and the claim is clear because $2 > \sqrt{3}$.

Third case: $\mathrm{ord}(\zeta) = 2n+1$ for some $n \in \mathbb{N}$. Then, ζ is a primitive root of unity, and thus $\mathrm{e}^{\frac{2\pi\mathrm{i}}{2n+1}} \in H$ implies $\mathrm{e}^{\frac{2n\pi\mathrm{i}}{2n+1}} \in H$. Now,

$$\frac{2n\pi}{2n+1} \,=\, \pi - \frac{\pi}{2n+1} \,\geqslant\, \pi - \frac{\pi}{3} \,=\, \frac{2\pi}{3}.$$

Using the fact that $-\cos(x)$ is increasing on the interval $[0,\pi]$, we get

$$\begin{aligned} \left|\mathrm{e}^{\frac{2n\pi\mathrm{i}}{2n+1}} - 1\right|^2 \,&=\, \Big[\cos\Big(\frac{2n\pi}{2n+1}\Big) - 1\Big]^2 + \Big[\sin\Big(\frac{2n\pi}{2n+1}\Big)\Big]^2 \\ &=\, 2 - 2\cos\Big(\frac{2n\pi}{2n+1}\Big) \,\geqslant\, 2 - 2\cos\Big(\frac{2\pi}{3}\Big) \,=\, 3, \end{aligned}$$

which proves the first claim, while the second claim is now obvious. □

We now show that, for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$, if one of the sets $\varLambda$ or $\varLambda^\varepsilon$ is relatively dense, the other one is uniformly discrete. The proof follows that of [30].

Proposition 5.6.6. *If $\varLambda \subseteq G$, one has the following properties.*

(i) *If $\varLambda$ is relatively dense, $\varLambda^\varepsilon$ is uniformly discrete for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(ii) *If $\varLambda^\varepsilon$ is relatively dense for some $0 < \varepsilon < \frac{\sqrt{3}}{2}$, the set $\varLambda$ is uniformly discrete.*

Proof. Claim (i). Let $K \subseteq G$ be compact with $\varLambda + K = G$. Pick ε' so that $2\varepsilon + \varepsilon' < \sqrt{3}$. Let $N(K,\varepsilon') := \big\{\chi \in \widehat{G} : |\chi(x) - 1| < \varepsilon' \text{ for all } x \in K\big\}$. Then, $N(K,\varepsilon')$ is an open neighbourhood of $1 \in \widehat{G}$; see page 182 for the notion of the underlying compact-open topology.

We prove that $(\varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon) \cap N(K,\varepsilon') = \{1\}$. Let $\chi \in (\varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon) \cap N(K,\varepsilon')$ and let $x \in G$. Then, by Lemma 5.6.4, we know that $\chi \in \varLambda^{2\varepsilon}$, and that $x = y + k$ for some $y \in \varLambda$ and $k \in K$. Hence

$$|\chi(x) - 1| \,=\, |\chi(y)\chi(k) - 1| \,\leqslant\, |\chi(y) - 1| + |\chi(k) - 1| \,\leqslant\, 2\varepsilon + \varepsilon' \,<\, \sqrt{3}.$$

As the image $\mathrm{im}(\chi) = \chi(G)$ is a subgroup of $\mathbb{S}^1$, we have $|z - 1| < \sqrt{3}$ for all $z \in \mathrm{im}(\chi)$. Then, Lemma 5.6.5 implies that $\mathrm{im}(\chi) = \{1\}$, which shows that $\chi = 1$, proving claim (i).

Claim (ii) follows immediately from (i) together with the observation that $\varLambda \subseteq (\varLambda^\varepsilon)^\varepsilon$; compare Eq. (5.6.1). □

Remark 5.6.7. In $\mathbb{R}^d$, the result in Proposition 5.6.6 holds for all $0 < \varepsilon < 1$; see [30, Prop. 6.5]. The reason why we get this stronger result is simple: If we pick any $0 < \varepsilon < 1$ with $\varepsilon' < 2 - 2\varepsilon$ and choose a $\chi \in (\varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon) \cap N(K,\varepsilon')$ exactly as in Proposition 5.6.6, we get

$$|\chi(x) - 1| \,\leqslant\, 2\varepsilon + \varepsilon' \tag{5.6.2}$$

for all $x \in G$. This shows that $-1 \notin \mathrm{im}(\chi)$.

If $G = \mathbb{R}^d$, then $\mathrm{im}(\chi)$ is a *connected* subgroup of $\mathbb{S}^1$ and thus is either $\{1\}$ or the entire $\mathbb{S}^1$. Therefore, $\mathrm{im}(\chi) = \{1\}$. $\Diamond$

Corollary 5.6.8. *If $\varLambda \subseteq G$ is relatively dense, the following properties hold.*

(i) *For all $0 < \varepsilon < \frac{\sqrt{3}}{4}$, the set $\varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon$ is uniformly discrete.*

(ii) *For all $0 < \varepsilon < \frac{\sqrt{3}}{6}$, the set $\varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon$ is uniformly discrete.*

Proof. We know that $\varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon \subseteq \varLambda^{2\varepsilon}$ and $\varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon \mathbin{\hat{-}} \varLambda^\varepsilon \subseteq \varLambda^{3\varepsilon}$. The proof then follows immediately from Proposition 5.6.6. □

Lemma 5.6.9. *Let $\varLambda \subseteq G$, define $\varDelta := \varLambda - \varLambda$, and let $\varepsilon > 0$. Then, one has $\varDelta \subseteq (\varLambda^\varepsilon)^{2\varepsilon}$ and $\varLambda^\varepsilon \subseteq \varDelta^{2\varepsilon}$.*

Proof. The first claim is a consequence of $\varDelta \subseteq (\varLambda^\varepsilon)^\varepsilon - (\varLambda^\varepsilon)^\varepsilon \subseteq (\varLambda^\varepsilon)^{2\varepsilon}$, compare Eq. (5.6.1), while the second follows from $\varLambda^\varepsilon \subseteq ((\varLambda^\varepsilon)^{2\varepsilon})^{2\varepsilon} \subseteq \varDelta^{2\varepsilon}$, where the final inclusion uses the first claim again. □

Corollary 5.6.10. *Let $\varLambda \subseteq G$. If, for some $0 < \varepsilon < \frac{\sqrt{3}}{4}$, the set $\varLambda^\varepsilon$ is relatively dense, then $\varLambda - \varLambda$ is uniformly discrete.*

Proof. Since $\varLambda^\varepsilon$ is relatively dense, and $2\varepsilon < \frac{\sqrt{3}}{2}$, it follows from Proposition 5.6.6(i) that $(\varLambda^\varepsilon)^{2\varepsilon}$ is uniformly discrete. By Lemma 5.6.9, the set $\varDelta = \varLambda - \varLambda$ is then also uniformly discrete. □

Theorem 5.6.11. *Let $\varLambda \subseteq G$ be relatively dense. If $\varLambda^\varepsilon$ is relatively dense for all $\varepsilon > 0$, then $\varLambda^\varepsilon$ is a model set for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

Proof. By Lemma 5.6.4, the family $\{\varLambda^\varepsilon\}_{0<\varepsilon<2}$ satisfies (A1) and (A3) in $\widehat{G}$. Since $\varLambda$ is relatively dense, Proposition 5.6.6 implies that $\varLambda^\varepsilon$ is also uniformly discrete for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$. Thus, $\{\varLambda^\varepsilon\}_{0<\varepsilon<\frac{\sqrt{3}}{2}}$ satisfies (A1)–(A4).

Moreover,

$$\bigcap_{\varepsilon'>0} \varLambda^{\varepsilon'} \;=\; \bigl\{\chi \in \widehat{G} : \chi(x) = 1 \text{ for all } x \in \varLambda\bigr\}.$$

Therefore, for any $\varepsilon > 0$, we have

$$\varLambda^\varepsilon \mathbin{\hat{+}} \bigcap_{\varepsilon'>0} \varLambda^{\varepsilon'} \;=\; \varLambda^\varepsilon.$$

The claim now follows from Corollary 5.2.9. □

Given a CPS $(\mathbb{R}^d, H, \mathcal{L})$, Meyer [29] and Moody [30] introduced a cut and project scheme in the dual spaces, called the *dual cut and project scheme*, and observed its importance in the study of the ε-dual sets of a Meyer set.

Theorem 5.6.12 ([41, Prop. 1])**.** *Let $(G, H, \mathcal{L})$ be a CPS. Then,*

$$\mathcal{Z} := \big\{(\chi, \psi) \in \widehat{G}\times\widehat{H} : \chi(s)\,\psi(y) = 1 \text{ for all } (x, y) \in \mathcal{L}\big\}.$$

is a lattice in $\widehat{G}\times\widehat{H}$, and $(\widehat{G}, \widehat{H}, \mathcal{Z})$ is a CPS. □

Let us note in passing that $\mathcal{Z}$ can also be viewed as the annihilator of the lattice $\mathcal{L}$ in $\widehat{G}\times\widehat{H} \cong \widehat{G\times H}$.

Definition 5.6.13. Given a CPS $(G, H, \mathcal{L})$, we call $(\widehat{G}, \widehat{H}, \mathcal{Z})$ from Theorem 5.6.12 the *dual CPS* to $(G, H, \mathcal{L})$.

Theorem 5.6.12 now implies the following result on ε-dual sets.

Proposition 5.6.14 ([46, Lemma 2.6])**.** *Let $\varLambda \subseteq G$ be a subset of a model set. Then, $\varLambda^{\varepsilon}$ is relatively dense for all $0 < \varepsilon < 2$.* □

Combining the results of this section, we obtain a (partial) characterisation of the subsets of model sets in general LCAGs, similar to [30, Thm. 9.1]. This characterisation will be completed in the next section in Theorem 5.7.8.

Theorem 5.6.15. *Let $\varLambda \subseteq G$ be relatively dense. Then, the following statements are equivalent.*

(i) *$\varLambda$ is a subset of a model set.*

(ii) *$\varLambda^{\varepsilon}$ is relatively dense for all $0 < \varepsilon < 2$.*

(iii) *$\varLambda^{\varepsilon}$ is a model set for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(iv) *$\varLambda^{\varepsilon}$ is a model set for some $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

Proof. The implication (i) $\Longrightarrow$ (ii) follows from Proposition 5.6.14 and (ii) $\Longrightarrow$ (iii) follows from Theorem 5.6.11, while (iii) $\Longrightarrow$ (iv) is obvious.

To complete the proof, we need to show that (iv) $\Longrightarrow$ (i). By Proposition 5.6.14, the set $(\varLambda^{\varepsilon})^{\varepsilon'}$ is relatively dense for any $0 < \varepsilon' < 2$. Since $\varLambda^{\varepsilon}$ is a model set, hence relatively dense, it follows from Theorem 5.6.11 that $(\varLambda^{\varepsilon})^{\varepsilon'}$ is a model set for all $0 < \varepsilon' < \frac{\sqrt{3}}{2}$. In particular, $(\varLambda^{\varepsilon})^{\varepsilon}$ is a model set, which contains the set $\varLambda$. □

Later, we will need to use the fact that, if $\varLambda$ is a set which satisfies one (and hence all) of the conditions in Theorem 5.6.15, then $t+\varLambda$ with $t \in G$ also satisfies the conditions of Theorem 5.6.15. We will give two different proofs of this fact, one in Corollary 5.6.18 based on the properties of the ε-dual sets, and another one in Proposition 5.6.19, using properties of model sets.

Lemma 5.6.16. *Let $\varLambda \subseteq G$, $\varepsilon > 0$ and $t \in G$. If $\varLambda^{\varepsilon}$ is relatively dense, then $(t + \varLambda)^{3\varepsilon}$ is relatively dense.*

PROOF. Select an integer n so that $\frac{2\pi}{n} < \varepsilon$. For every $0 \leqslant k \leqslant n-1$, let $C_k := \left\{ \mathrm{e}^{\mathrm{i}\theta} : \frac{2k\pi}{n} \leqslant \theta < \frac{2(k+1)\pi}{n} \right\}$. Then, $\bigcup_{k=0}^{n-1} C_k$ is a partition of $\mathbb{S}^1$. Define

$$\varGamma_k \,:=\, \{\chi \in \varLambda^\varepsilon : \chi(t) \in C_k\}.$$

It is clear by construction that

$$\varLambda^\varepsilon \,=\, \bigcup_{k=0}^{n-1} \varGamma_k.$$

We now show that

$$\varGamma_k \mathbin{\hat{-}} \varGamma_k \,\subseteq\, (t+\varLambda)^{3\varepsilon}.$$

Let $\chi_1, \chi_2 \in \varGamma_k$, and $x \in \varLambda$ be arbitrary. Then,

$$\begin{aligned}
\left|\chi_1(t+x)\overline{\chi_2(t+x)} - 1\right| \,&=\, \left|\chi_1(t)\overline{\chi_2(t)}\chi_1(x)\overline{\chi_2(x)} - 1\right| \\
&\leqslant\, \left|\chi_1(t)\overline{\chi_2(t)}\chi_1(x)\overline{\chi_2(x)} - \chi_1(x)\overline{\chi_2(x)}\right| \\
&\qquad + \left|\chi_1(x)\overline{\chi_2(x)} - \overline{\chi_2(x)}\right| + \left|\overline{\chi_2(x)} - 1\right| \\
&=\, \left|\chi_1(t)\overline{\chi_2(t)} - 1\right| + \left|\chi_1(x) - 1\right| + \left|\overline{\chi_2(x)} - 1\right| \\
&\leqslant\, \left|\chi_1(t)\overline{\chi_2(t)} - 1\right| + 2\varepsilon.
\end{aligned}$$

Since $\chi_1, \chi_2 \in \varGamma_k$, we have $(\chi_1 \mathbin{\hat{-}} \chi_2)(t) = \chi_1(t)\overline{\chi_2(t)} \in \left\{ \mathrm{e}^{\mathrm{i}\theta} : -\frac{2\pi}{n} \leqslant \theta \leqslant \frac{2\pi}{n} \right\}$, and hence

$$\left|\chi_1(t)\overline{\chi_2(t)} - 1\right| \,\leqslant\, \frac{2\pi}{n} < \varepsilon.$$

Consequently,

$$\left|\chi_1(t+x)\overline{\chi_2(t+x)} - 1\right| \,<\, 3\varepsilon.$$

Let now $K \subseteq \widehat{G}$ be any compact set so that $\varLambda^\varepsilon \mathbin{\hat{+}} K = \widehat{G}$. Define the set $J := \{k : 0 \leqslant k \leqslant n-1, \varGamma_k \neq \varnothing\}$. For each $j \in J$, pick some $\chi_j \in \varGamma_j$. Then,

$$\begin{aligned}
\widehat{G} \,&\subseteq\, \bigcup_{k=0}^{n-1} (\varGamma_k \mathbin{\hat{+}} K) \,=\, \bigcup_{j\in J} (\varGamma_j \mathbin{\hat{+}} K) \,=\, \bigcup_{j\in J} (\mathbin{\hat{-}}\chi_j \mathbin{\hat{+}} \varGamma_j \mathbin{\hat{+}} \chi_j \mathbin{\hat{+}} K) \\
&\subseteq\, \bigcup_{j\in J} (\varGamma_j \mathbin{\hat{-}} \varGamma_j \mathbin{\hat{+}} \chi_j \mathbin{\hat{+}} K) \\
&\subseteq\, \bigcup_{j\in J} \left[(t+\varLambda)^{3\varepsilon} \mathbin{\hat{+}} \chi_j \mathbin{\hat{+}} K\right] \,=\, (t+\varLambda)^{3\varepsilon} \mathbin{\hat{+}} \bigcup_{j\in J} (\chi_j \mathbin{\hat{+}} K).
\end{aligned}$$

As $\bigcup_{j\in J} (\chi_j \mathbin{\hat{+}} K)$ is compact, we are done. □

Remark 5.6.17. The result of Lemma 5.6.16 can easily be improved as follows. Let $\varepsilon' > 0$. If one picks n so that $\frac{2\pi}{n} < \varepsilon$, the same proof yields that $(t+\varLambda)^{2\varepsilon+\varepsilon'}$ is relatively dense. ◊

An immediate consequence of Lemma 5.6.16 is the following result.

Corollary 5.6.18. *Let $\varLambda \subseteq G$ be relatively dense and $t \in G$. Then, the following statements are equivalent.*

(i) *$\varLambda^{\varepsilon}$ is relatively dense for all $0 < \varepsilon < 2$.*

(ii) *$(t+\varLambda)^{\varepsilon}$ is relatively dense for all $0 < \varepsilon < 2$.* □

Note that, for any $\varnothing \neq \varGamma \subseteq G$ and any $\varepsilon \geqslant 2$, we have $\varGamma^{\varepsilon} = \widehat{G}$. Thus, $\varGamma^{\varepsilon}$ is trivially relatively dense for all $\varepsilon \geqslant 2$.

As mentioned earlier, Corollary 5.6.18 may also be obtained by combining Theorem 5.6.15 with the following result.

Proposition 5.6.19. *Let $\varLambda \subseteq G$ be a subset of a model set and let $F \subseteq G$ be a finite non-empty set. Then, $\varLambda + F$ is a subset of a model set.*

Proof. Let $\curlywedge(W)$ be any model set containing $\varLambda$, and let $(G, H, \mathcal{L})$ be its CPS. The problem we face is that F might not be in the projection of the lattice, thus we will need to enlarge the lattice in the CPS.

Let $K \subseteq H$ be any compact set so that $W \cup \{0\} \subseteq K^{\circ}$. Let $g \in C_{\mathsf{c}}(G)$ be such that $g(x) = 1$ for all $x \in K$. Let $\omega = \omega_g$. Then, ω is norm-almost periodic and $\mathrm{supp}(\omega)$ is a model set.

Let now $L' := \langle \mathrm{supp}(\omega) \cup F \rangle$. Then, the pair $\big(\{P^{\infty}_{\varepsilon}(\omega)\}_{0<\varepsilon<\|\omega\|_{\infty}}, L'\big)$ satisfies conditions (A1)–(A5). By Corollary 5.4.4, we thus obtain a CPS in which the sets $\{P^{\infty}_{\varepsilon}(\omega)\}_{0<\varepsilon<\|\omega\|_{\infty}}$ are model sets.

Let W_0 be the window of one such $P^{\infty}_{\varepsilon}(\omega)$ and consider the supporting set $\varGamma := \mathrm{supp}(\omega) \subseteq L'$. Then, $\curlywedge(W_0) \subseteq \varGamma \subseteq L'$, and $\varGamma$ is a model set, hence has finite local complexity. Therefore, by Lemma 5.5.1, there exists a finite set $J \subseteq G$ so that

$$\varGamma \subseteq \curlywedge(W_0) + J .$$

Since L' is a group which contains both $\curlywedge(W_0)$ and $\varGamma$, it is easy to see that the smallest such J is also a subset of L'. We can thus define $J^{\star} := \{j^{\star} : j \in J\}$. Then,

$$\varLambda \subseteq \varGamma \subseteq \curlywedge(W + J^{\star}) ,$$

and, since $F \subseteq L'$,

$$\varLambda + F \subseteq \curlywedge(W + J^{\star} + F^{\star}) .$$

Thus, $\varLambda + F$ is relatively dense and is a subset of a model set. □

5.7. Almost lattices

In this section, we complete the characterisation of Meyer sets by studying the so-called almost lattice property; see Definition 5.7.2 below. We start by reviewing a result from [29]. As this result is not stated explicitly there, and the details are somewhat lost along the way, we include it with a proof.

Lemma 5.7.1. *Let $\varLambda \subseteq G$ be relatively dense. Then, the following statements are equivalent.*

(i) *$\varLambda - \varLambda - \varLambda$ is locally finite.*

(ii) *$\varLambda - \varLambda - \varLambda$ is uniformly discrete.*

(iii) *$\varLambda$ is locally finite and there exists a finite set F so that $\varLambda - \varLambda \subseteq \varLambda + F$.*

Proof. The implication (ii) $\Longrightarrow$ (i) is obvious.

Let us now show that (i) $\Longrightarrow$ (iii). Since $\varLambda$ is relatively dense, there exists a compact set $K \subseteq G$ so that $\varLambda + K = G$. Let

$$F := (\varLambda - \varLambda - \varLambda) \cap K,$$

which is a finite set. We now prove that $\varLambda - \varLambda \subseteq \varLambda + F$, which completes this implication.

Let $y \in \varLambda - \varLambda$. Then $y \in G = \varLambda + K$, and thus $y = z + k$ for some $z \in \varLambda$ and $k \in K$. Then, $k = y - z$ and therefore $k \in \varLambda - \varLambda - \varLambda$. This shows that $k \in F$, and since $z \in \varLambda$, we are done.

Finally, to show that (iii) $\Longrightarrow$ (ii), note that

$$\varLambda - \varLambda - \varLambda \subseteq (\varLambda + F) - \varLambda \subseteq \varLambda + F + F.$$

Hence

$$\begin{aligned}(\varLambda - \varLambda - \varLambda) - (\varLambda - \varLambda - \varLambda) &\subseteq (\varLambda + F + F) - (\varLambda + F + F)\\ &= (\varLambda - \varLambda) + F + F - F - F\\ &\subseteq \varLambda + F + F + F - F - F.\end{aligned}$$

Since $\varLambda$ is locally finite and F is finite, the set $\varLambda + F + F + F - F - F$ is locally finite, and hence there exists an open neighbourhood U of $0 \in G$ so that $(\varLambda + F + F + F - F - F) \cap U = \{0\}$. Then, $\varLambda - \varLambda - \varLambda$ is U-uniformly discrete. □

Let us next recall the definition of an almost lattice from [29, 30].

Definition 5.7.2. Let $\varLambda \subseteq G$. We say that $\varLambda$ is an *almost lattice* if $\varLambda$ is locally finite and relatively dense and if there exists a finite set F such that $\varLambda - \varLambda \subseteq \varLambda + F$.

An important property of almost lattices, which will carry on to Meyer sets, is that they are closed under taking Minkowski differences. We show this in the next lemma. This property is the key to Theorem 5.7.7, which later will allow us to complete the general characterisation of Meyer sets.

Lemma 5.7.3. *Let $\varLambda \subseteq G$ be an almost lattice. Then, $\varLambda - \varLambda$ is also an almost lattice. In particular, any almost lattice has finite local complexity.*

PROOF. If $\varLambda$ is an almost lattice, then $\varLambda - \varLambda \subseteq \varLambda + F$ is locally finite. Also, $\varLambda - \varLambda$ contains a translate of $\varLambda$ and thus is relatively dense. Moreover,

$$(\varLambda - \varLambda) - (\varLambda - \varLambda) \subseteq (\varLambda - \varLambda) + F - F,$$

where $F - F$ is still a finite set. □

In the proof of Theorem 5.7.7 below, we will need to use the autocorrelation measure. We start by reviewing the definition and properties of autocorrelation measures. For a more detailed overview, we refer the reader to [AO1, Sec. 9.1.1] for $G = \mathbb{R}^d$ and to [14, 24] for the general case. Let us begin with an important concept; compare [AO1, Def. 2.9 and Rem. 2.5].

Definition 5.7.4. A sequence of compact measurable subsets $B_n \subseteq G$ is called a *van Hove sequence* if, for every compact set $K \subseteq G$, we have

$$\lim_{n\to\infty} \frac{\theta_G(\partial^K(B_n))}{\theta_G(B_n)} = 0,$$

where the *K-boundary* $\partial^K(B_n)$ of B_n is defined as

$$\partial^K(B_n) := \big(((K + B_n) \setminus B_n^\circ) \cup ((-K + \overline{G \setminus B_n}) \cap B_n)\big),$$

and the bar (circle) denotes the closure (interior) of the set; compare also Eq. (4.1.3).

Now, given a translation bounded measure ω and a van Hove sequence B_n, we can define a sequence γ_n via

$$\gamma_n := \frac{\omega_{B_n} * \widetilde{\omega_{B_n}}}{\theta_G(B_n)},$$

where ω_{B_n} denotes the restriction $1_{B_n}\omega$ of ω to the set B_n, while $\widetilde{\ }$ and the convolution $*$ are recalled in Sections 4.1.2 and 4.3.4 as well as in Definition 4.9.18; see [AO1, Chs. 8 and 9] for more.

As ω is translation bounded and the sets B_n are compact, the measures γ_n are well defined. Moreover, the sequence $\{\gamma_n\}$ is precompact in the vague topology[11] [14, Prop. 2.2] (compare [AO1, Prop. 9.1] for $G = \mathbb{R}^d$), hence it has cluster points, and every cluster point is a translation bounded measure.

Definition 5.7.5. Given a translation bounded measure ω and a van Hove sequence B_n, every cluster point γ of γ_n is called an *autocorrelation measure* of ω.

It is easy to see that each γ_n is a positive definite measure, and therefore every autocorrelation measure γ is a positive definite measure (see Section 4.11 in this volume for the definition and properties of positive definite

[11] See [35] for the definition of the vague topology for measures; compare also page 209 in Chapter 4 and [AO1, Sec. 8.5.1].

measures, and [AO1, Ch. 9] for further details). Let us also note that, if γ is an autocorrelation of ω, then there exists a subsequence B_{k_n} of B_n such that, in the vague topology, we have $\gamma = \lim_n \gamma_{k_n}$. Therefore, $A_n := B_{k_n}$ is a van Hove sequence and

$$\gamma := \lim_n \frac{\omega_{A_n} * \widetilde{\omega_{A_n}}}{\theta_G(A_n)}.$$

Definition 5.7.6. We define an *autocorrelation measure* of a Delone set $\varLambda \subseteq G$ as an autocorrelation of the corresponding Dirac comb $\delta_\varLambda = \sum_{x\in\varLambda} \delta_x$.

Next, we prove that every almost lattice is a subset of a model set. The key for this theorem is a result from [28] which shows that the autocorrelation measure of a weakly almost periodic measure is strongly almost periodic. Therefore, if $\varLambda$ is an almost lattice with autocorrelation γ, and if η is the autocorrelation measure of γ, then η is a strongly almost periodic measure supported on an almost lattice. Thus, we can apply Theorem 5.5.2, and the claim follows from there.

Theorem 5.7.7. *Let G be a σ-compact LCAG, and let $\varLambda \subseteq G$ be an almost lattice. Then, $\varLambda$ is a subset of a model set.*

Proof. Let γ be an autocorrelation for $\varLambda$. Since $\varLambda$ is relatively dense, $\gamma \neq 0$. Also, since $\varLambda$ has finite local complexity, γ is a pure point measure with $\operatorname{supp}(\gamma) \subseteq \varLambda - \varLambda$.

Let η be an autocorrelation of γ. Here, γ is a translation bounded and positive definite measure and is thus weakly almost periodic by Corollary 4.11.6. We now repeat the argument of [47, 28] to show that η is also strongly almost periodic.

For all $f, g \in C_{\mathsf{c}}(G)$, the functions $f * \gamma$ and $g * \widetilde{\gamma}$ are weakly almost periodic functions. Their Eberlein convolution[12] $(f * \gamma) \star (g * \widetilde{\gamma})$ is thus a strongly almost periodic function by Theorem 4.6.3. An easy computation shows that $(f * \gamma) \star (g * \widetilde{\gamma}) = f * g * \eta$. Indeed, for any fixed $t \in G$, we have

$$\begin{aligned}\big((f * \gamma) \star (g * \widetilde{\gamma})\big)(t) &= \lim_{n\to\infty} \frac{\int_{A_n} (f * \gamma)(s)\, (g * \widetilde{\gamma})(t - s)\, \mathrm{d}\theta_G(s)}{\theta_G(A_n)} \\ &= \lim_{n\to\infty} \frac{\int_G (f * \gamma)(s)\, (g * \widetilde{\gamma})(t - s)\, 1_{A_n}(s)\, \mathrm{d}\theta_G(s)}{\theta_G(A_n)}.\end{aligned}$$

By [5, Lemma 5] or [40, Lemma 1.2], we get

$$f * \eta * g = \lim_{n\to\infty} \frac{f * \gamma_{A_n} * \widetilde{\gamma} * g}{\theta_G(A_n)},$$

[12] See Definition 4.6.1 for the notion and [AO1, Sec. 8.8] for more on the case $G = \mathbb{R}^d$, where the symbol $\circledast$ is used for the Eberlein convolution.

and thus we obtain

$$
\begin{aligned}
&\big|\big((f*\gamma)\star(g*\widetilde{\gamma})\big)(t)-(f*g*\eta)(t)\big| \\
&= \Big|\lim_{n\to\infty}\frac{\int_G (f*\gamma)(s)\,(g*\widetilde{\gamma})(t-s)\,1_{A_n}(s)\,\mathrm{d}\theta_G(s)}{\theta_G(A_n)} \\
&\qquad -\lim_{n\to\infty}\frac{\int_G (f*\gamma_{A_n})(s)\,(g*\widetilde{\gamma})(t-s)\,\mathrm{d}\theta_G(s)}{\theta_G(A_n)}\Big| \\
&\leqslant \lim_{n\to\infty}\frac{\int_G \big|(f*\gamma)(s)\,1_{A_n}(s)\,(g*\widetilde{\gamma})(t-s)-(f*\gamma_{A_n})(s)\,(g*\widetilde{\gamma})(t-s)\big|\,\mathrm{d}\theta_G(s)}{\theta_G(A_n)} \\
&= \lim_{n\to\infty}\frac{\int_G \big|(f*\gamma)(s)\,1_{A_n}(s)-(f*\gamma_{A_n})(s)\big|\,\big|(g*\widetilde{\gamma})(t-s)\big|\,\mathrm{d}\theta_G(s)}{\theta_G(A_n)} \\
&\leqslant \lim_{n\to\infty}\|g*\widetilde{\gamma}\|_\infty\frac{\int_G \big|(f*\gamma)(s)\,1_{A_n}(s)-(f*\gamma_{A_n})(s)\big|\,\mathrm{d}\theta_G(s)}{\theta_G(A_n)}.
\end{aligned}
$$

Let $K\subseteq G$ be any compact set containing $\pm\operatorname{supp}(f)$. We claim that

$$
(f*\gamma)(s)\,1_{A_n}(s)-(f*\gamma_{A_n})(s)\neq 0 \implies s\in\partial^K(A_n).
$$

We need to consider two cases. Start with the case that $s\in A_n$. Then,

$$
(f*\gamma)(s)\neq(f*\gamma_{A_n})(s)\implies\int_G f(s-t)\,\mathrm{d}\gamma(t)\neq\int_G f(s-t)\,1_{A_n}(t)\,\mathrm{d}\gamma(t),
$$

which implies that

$$
\int_G f(s-t)\,(1-1_{A_n}(t))\,\mathrm{d}\gamma(t)=\int_{G\setminus A_n} f(s-t)\,\mathrm{d}\gamma(t)\neq 0.
$$

Consequently, there must be a $t\notin A_n$ such that $f(s-t)\neq 0$, which means that $s-t\in\operatorname{supp}(f)$. Therefore, $s\in(G\setminus A_n)+K$. Since $s\in A_n$, we get $s\in\partial^K(A_n)$.

Now, consider the case that $s\notin A_n$. Then,

$$
0\neq\big(f*\gamma_{A_n}\big)(s)=\int_G f(s-t)\,1_{A_n}(t)\,\mathrm{d}\gamma(t).
$$

Consequently, there exists a t so that $f(s-t)\,1_{A_n}(t)\neq 0$. Hence, $t\in A_n$ and $s-t\in\operatorname{supp}(f)$. This shows that $s\in A_n+K$, and therefore $s\in\partial^K(A_n)$.

Now, since $(f * \gamma)(s)\, 1_{A_n}(s) - (f * \gamma_{A_n})(s) = 0$ for s outside $\partial^K(A_n)$, we get

$$\begin{aligned}
&\big|\big((f * \gamma) \star (g * \widetilde{\gamma})\big)(t) - (f * g * \eta)(t)\big| \\
&\qquad \leqslant \lim_{n\to\infty} \|g * \widetilde{\gamma}\|_\infty \frac{\int_G \big|(f * \gamma)(s)\, 1_{A_n}(s) - (f * \gamma_{A_n})(s)\big| \,\mathrm{d}\theta_G(s)}{\theta_G(A_n)} \\
&\qquad = \|g * \widetilde{\gamma}\|_\infty \lim_{n\to\infty} \frac{\int_{\partial^K(A_n)} \big|(f * \gamma)(s)\, 1_{A_n}(s) - (f * \gamma_{A_n})(s)\big| \,\mathrm{d}\theta_G(s)}{\theta_G(A_n)} \\
&\qquad \leqslant \|g * \widetilde{\gamma}\|_\infty \lim_{n\to\infty} \frac{\int_{\partial^K(A_n)} 2\,\|f * \gamma\|_\infty \,\mathrm{d}\theta_G(s)}{\theta_G(A_n)} \\
&\qquad = 2\|f * \gamma\|_\infty \, \|g * \widetilde{\gamma}\|_\infty \lim_{n\to\infty} \frac{\theta_G(\partial^K A_n)}{\theta_G(A_n)} \;=\; 0,
\end{aligned}$$

where the last step is a consequence of the van Hove property. Thus, for any $f, g \in C_{\mathsf{c}}(G)$, the function $f * g * \eta$ is almost periodic. Therefore, by Proposition 4.10.3, η is a strongly almost periodic measure.

Since $\varLambda$ is an almost lattice, we have $\mathrm{supp}(\eta) \subseteq (\varLambda - \varLambda) - (\varLambda - \varLambda) =: \varGamma$ and $\varGamma$ is an almost lattice. Therefore, η is a strongly almost periodic measure and $\mathrm{supp}(\eta) - \mathrm{supp}(\eta)$ is uniformly discrete. Thus, by Theorem 5.5.2, $\mathrm{supp}(\eta)$ is a model set.

As $\mathrm{supp}(\eta) \subseteq \varGamma$ and $\varGamma$ has finite local complexity, Lemma 5.5.1 implies that there exists a finite set $J \subseteq G$ such that

$$\varGamma \;\subseteq\; \mathrm{supp}(\eta) + J.$$

For some $x \in \varLambda$, we thus have

$$\varLambda - x \;=\; \varLambda - x + x - x \;\subseteq\; (\varLambda - \varLambda) - (\varLambda - \varLambda) \;\subseteq\; \mathrm{supp}(\eta) + J.$$

By Proposition 5.6.19, $\varLambda$ is then a subset of a model set. □

We can now complete our characterisation of Meyer sets in a general LCAG, which is similar to the characterisation of Meyer sets in $\mathbb{R}^d$ given in [30, Thm. 9.1].

Theorem 5.7.8. *Let $\varLambda \subseteq G$ be relatively dense, where G is a σ-compact LCAG. Then, the following properties are equivalent.*

(i) *$\varLambda$ is a subset of a model set.*

(ii) *$\varLambda^{\varepsilon}$ is relatively dense for all $0 < \varepsilon < 2$.*

(iii) *$\varLambda^{\varepsilon}$ is a model set for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(iv) *$\varLambda^{\varepsilon}$ is a model set for some $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(v) *$\varLambda^{\varepsilon}$ is relatively dense for some $0 < \varepsilon < \frac{\sqrt{3}}{6}$.*

(vi) *$\varLambda$ is an almost lattice.*

(vii) $\Lambda - \Lambda - \Lambda$ *is locally finite.*

PROOF. The equivalences (i) $\iff$ (ii) $\iff$ (iii) $\iff$ (iv) follow from Theorem 5.6.15. The equivalence (vi) $\iff$ (vii) follows from Lemma 5.7.1.

The implications (iii) $\implies$ (v) and (i) $\implies$ (vii) are trivial, while the implication (vi) $\implies$ (i) follows from Theorem 5.7.7.

We now show (v) $\implies$ (i) to complete the proof. Since $\Lambda^\varepsilon \doteq \Lambda^\varepsilon \doteq \Lambda^\varepsilon \subseteq \Lambda^{3\varepsilon}$ and $3\varepsilon < \frac{\sqrt{3}}{2}$, it follows from Proposition 5.6.6 that $\Lambda^\varepsilon \doteq \Lambda^\varepsilon \doteq \Lambda^\varepsilon$ is uniformly discrete. Also, according to property (v), Λ^ε is relatively dense.

Thus, Λ^ε is an almost lattice by Lemma 5.7.1, and hence, by Theorem 5.7.7, Λ^ε is a subset of a model set. Then, by Theorem 5.6.15, $(\Lambda^\varepsilon)^\varepsilon$ is a model set which contains Λ. □

Let us finally recall the general definition of a Meyer set.

Definition 5.7.9. A set $\Lambda \subseteq G$ is called a *Meyer set* if Λ is relatively dense and $\Lambda - \Lambda - \Lambda$ is locally finite.

For a relatively dense subset Λ of a σ-compact LCAG G, any of the seven conditions in Theorem 5.7.8 is equivalent to Λ being a Meyer set.

The following result follows immediately from the properties of almost lattices and model sets.

Corollary 5.7.10. *Let $\Lambda \subseteq G$ be a Meyer set and F be a finite set. Then, $\Lambda + F$, $\Lambda \cup F$ and $\Lambda \pm \Lambda \pm \ldots \pm \Lambda$ are Meyer sets. In particular, $\Delta := \Lambda - \Lambda$ is a Meyer set.* □

In the case of a metrisable LCAG, it follows from Theorem 5.A.2 in the Appendix that we can add one more characterisation, namely that of Λ being harmonious, to Theorem 5.7.8. We refer the reader to the Appendix for the definition and properties of harmonious sets.

Theorem 5.7.11. *Let G be a metrisable σ-compact LCAG and let $\Lambda \subseteq G$ be relatively dense. Then, the following properties are equivalent.*

(i) *Λ is a subset of a model set.*

(ii) *Λ^ε is relatively dense for all $0 < \varepsilon < 2$.*

(iii) *Λ^ε is a model set for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(iv) *Λ^ε is a model set for some $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(v) *Λ^ε is relatively dense for some $0 < \varepsilon < \frac{\sqrt{3}}{6}$.*

(vi) *Λ is an almost lattice.*

(vii) *$\Lambda - \Lambda - \Lambda$ is locally finite.*

(viii) *Λ is harmonious.* □

In the case of compactly generated[13] LCAGs, Baake, Lenz and Moody showed [6] that the condition that $\varLambda$ *is an almost lattice* is equivalent to the weaker condition that $\varLambda - \varLambda$ *is weakly uniformly discrete*. Thus, we also obtain the following result.

Theorem 5.7.12. *Let G be a compactly generated LCAG and let $\varLambda \subseteq G$ be relatively dense. Then, the following statements are equivalent.*

(i) *$\varLambda$ is a subset of a model set,*
(ii) *$\varLambda^{\varepsilon}$ is relatively dense for all $0 < \varepsilon < 2$,*
(iii) *$\varLambda^{\varepsilon}$ is a model set for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$,*
(iv) *$\varLambda^{\varepsilon}$ is a model set for some $0 < \varepsilon < \frac{\sqrt{3}}{2}$,*
(v) *$\varLambda^{\varepsilon}$ is relatively dense for some $0 < \varepsilon < \frac{\sqrt{3}}{6}$,*
(vi) *$\varLambda$ is an almost lattice,*
(vii) *$\varLambda - \varLambda$ is weakly uniformly discrete.*

Proof. In this case, the implication (vii) $\Longrightarrow$ (vi) was proved in [6, Thm. 11]. The rest of the theorem now follows from Theorem 5.7.8. □

5.8. WAP measures with Meyer set support

Here, we study the properties of weakly almost periodic measures supported inside Meyer sets. The key tool for this section is Corollary 5.8.2 below, which states that the class of weakly almost periodic measures supported inside a Meyer set is closed under the canonical almost periodic decomposition. Our results have important consequences for the diffraction of measures supported inside Meyer sets. The latter will be considered in Section 5.9.

For the definition of weak almost periodicity for measures, and the Eberlein decomposition

$$\mu \,=\, \mu_{\mathsf{s}} + \mu_0$$

of a weakly almost periodic measure into its strongly and null-weakly almost periodic components, we refer the reader to Section 4.10.

We start by reviewing a result of [46], which shows the stability of the class of weighted Dirac combs supported inside Meyer sets under the Eberlein decomposition. Similar results have recently been obtained via a dynamical systems approach in [2, 28].

Theorem 5.8.1 ([46, Thm. 4.6])**.** *Let $(G, H, \mathcal{L})$ be a CPS, let $W \subseteq H$ be a compact set and let μ be a weakly almost periodic measure such that* $\mathrm{supp}(\mu) \subseteq \curlywedge(W)$. *Then,* $\mathrm{supp}(\mu_{\mathsf{s}}) \subseteq \curlywedge(W)$ *and* $\mathrm{supp}(\mu_0) \subseteq \curlywedge(W)$. □

[13] Up to isomorphisms, these are the groups of the form $\mathbb{R}^d \times \mathbb{Z}^n \times \mathbb{K}$ for some $d, n \in \mathbb{N}_0$ and some compact Abelian group $\mathbb{K}$; see [13, Thm. 9.8].

An immediate consequence of Theorem 5.8.1 is the following result.

Corollary 5.8.2. *Let μ be a weakly almost periodic measure in some σ-compact LCAG such that* $\operatorname{supp}(\mu)$ *is a subset of a Meyer set. Then,* $\operatorname{supp}(\mu_{\mathsf{s}})$ *and* $\operatorname{supp}(\mu_0)$ *are also subsets of Meyer sets.*

Proof. Let $\varLambda$ be a Meyer set such that $\operatorname{supp}(\mu) \subseteq \varLambda$. By Theorem 5.7.8, there exists some model set $\curlywedge(W)$ such that $\varLambda \subseteq \curlywedge(W)$. As $\overline{W}$ is compact and $\operatorname{supp}(\mu) \subseteq \curlywedge(\overline{W})$, it follows from Theorem 5.8.1 that $\operatorname{supp}(\mu_{\mathsf{s}})$ and $\operatorname{supp}(\mu_0)$ are subsets of the Meyer set $\curlywedge(\overline{W})$. □

It follows from Corollary 5.8.2 that, given a weakly almost periodic measure μ whose support is a subset of a Meyer set, the strongly almost periodic component μ_{s} satisfies condition (iii), and hence all the conditions, of Theorem 5.5.2. In [43, Prop. 5.7], it was observed that null-weakly almost periodic measures supported inside Meyer sets are also easy to characterise. Combining these observations leads to a simple characterisation of the decomposition of almost periodic measures with Meyer set support. In the current setting, we require a more general version of an equivalence given in [43, Prop. 5.7]. To obtain this, we need two preliminary results.

We first prove that, if we have a measure with uniformly discrete support, the absolute value of the convolution between the measure and a function with a small support is exactly the convolution between the absolute value of the function and the total variation of the measure.

Lemma 5.8.3. *Let μ be a pure point Radon measure with U-uniformly discrete support, and let f be a function with* $\operatorname{supp}(f) \subseteq U$. *Then,*

$$|f * \mu| \,=\, |f| * |\mu| \,.$$

Proof. Let $\varGamma = \operatorname{supp}(\mu)$. For all $x \in G$, we have

$$|f * \mu|\,(x) \,=\, \Bigl| \sum_{t \in \varGamma} f(x+t) \mu(\{t\}) \Bigr|$$

and

$$\bigl(|f| * |\mu|\bigr)(x) \,=\, \sum_{t \in \varGamma} |f(x+t)|\, |\mu(\{t\})| \,.$$

Now, if $t_1, t_2 \in \varGamma$ are such that $f(x+t_1) \neq 0$ and $f(x+t_2) \neq 0$, then $x+t_1, x+t_2 \in \operatorname{supp}(f) \subseteq U$, and hence

$$-x \in (t_1 - U) \cap (t_2 - U).$$

By uniform discreteness, we get that $t_1 = t_2$. This shows that each of the sums $\sum_{t \in \varGamma} f(x+t)\mu(\{t\})$ and $\sum_{t \in \varGamma} |f(x+t)|\, |\mu(\{t\})|$ contains at most one non-zero term, and the claim follows. □

Next, we prove that the total variation measure of a weakly almost periodic measure with uniformly discrete support is also weakly almost periodic.

Lemma 5.8.4. *Let μ be a pure point Radon measure with uniformly discrete support. If μ is weakly (strongly) almost periodic, $|\mu|$ is also weakly (strongly) almost periodic.*

Proof. We only show the argument for weak almost periodicity, because the other case is completely analogous.

Let U be an open set so that $\mathrm{supp}(\mu)$ is U-uniformly discrete, and define

$$S := \big\{ f \in C_{\mathsf{c}}(G) : f \geqslant 0 \text{ and } \mathrm{supp}(f) \subset U \big\}.$$

Then, for all $f \in S$, the function $f * \mu$ is weakly almost periodic, and therefore so is $|f * \mu| = f * |\mu|$; see Proposition 4.3.11 (or Corollary 4.3.6 for the case of strong almost periodicity).

This shows that $f * |\mu|$ is weakly almost periodic for all f in S. Because the space of almost periodic functions is closed under translations, we can conclude that $f * |\mu|$ is a weakly almost periodic function for all functions $f \in \mathcal{O}_S := \{T_t g : g \in S, t \in G\}$.

As any function $g \in C_{\mathsf{c}}(G)$ can be written as a finite linear combination of functions in $\mathcal{O}_S$, the claim follows. □

Remark 5.8.5. The converse of Lemma 5.8.4 is not true. Indeed, consider the weighted Thue–Morse comb ω with weights $\{\pm 1\}$; see [AO1, Sec. 10.1]. The variation measure of this comb is $\delta_{\mathbb{Z}}$, which is a strongly almost periodic measure. But ω cannot be a weakly almost periodic measure, as this would imply that ω has pure point diffraction [28]. ♢

An immediate consequence of Lemma 5.8.4 is the following corollary.

Corollary 5.8.6. *Let μ be a weakly almost periodic measure with uniformly discrete support in some σ-compact LCAG G, and let $\{A_n\}$ be a van Hove sequence. Then, the following statements are equivalent,*

(i) *μ is null-weakly almost periodic;*
(ii) *$|\mu|$ is null-weakly almost periodic;*
(iii) $\lim_{n\to\infty} \frac{|\mu|(A_n)}{\theta_G(A_n)} = 0$.

Proof. By Lemma 5.8.4, we know that $|\mu|$ is also a weakly almost periodic measure. Therefore, by Lemma 4.10.7, the limit

$$\lim_{n\to\infty} \frac{|\mu|(A_n)}{\theta_G(A_n)}$$

exists and is equal to $M(|\mu|)$.

The equivalence (ii) $\iff$ (iii) follows immediately from the observation that a positive weakly almost periodic measure is null-weakly almost periodic if and only if it has zero mean, in conjunction with Lemma 4.10.7.

We next prove (i) $\implies$ (iii). Let U be any open set such that $\operatorname{supp}(\mu)$ is U-uniformly discrete, and let $0 \not\equiv f \in C_{\mathsf{c}}(G)$ be such that $\operatorname{supp}(f) \subset U$ and $f \geqslant 0$. Then, by Lemma 5.8.3, we have $|f * \mu| = f * |\mu|$. Therefore, by Lemma 4.10.7, we have

$$\left(\int_G f(x)\,\mathrm{d}x\right) M\big(|\mu|\big) \,=\, M\big(f * |\mu|\big) \,=\, M\big(|f * \mu|\big) \,=\, 0.$$

We complete the proof by showing that (iii) $\implies$ (i). Let $f \in C_{\mathsf{c}}(G)$. Then, as μ and $|\mu|$ are weakly almost periodic, the functions $f * \mu$ and $|f| * |\mu|$ are weakly almost periodic as well. It follows from Proposition 4.3.11 that $|f * \mu|$ is also a weakly almost periodic function. Therefore, $f * \mu, |f * \mu|$ and $|f| * |\mu|$ are amenable by Proposition 4.5.9.

We now have

$$M\big(|f * \mu|\big) \,\leqslant\, M\big(|f| * |\mu|\big) \,=\, \left(\int_G |f(x)|\,\mathrm{d}x\right) M\big(|\mu|\big) \,=\, 0,$$

which completes the proof. □

Combining Corollary 5.8.2, Theorem 5.5.2 and Corollary 5.8.6, we get the following result.

Proposition 5.8.7. *Let μ be a weakly almost periodic measure on some σ-compact LCAG G such that* $\operatorname{supp}(\mu)$ *is a subset of a Meyer set, and let $\{A_n\}$ be a van Hove sequence. Then, one has*

(i) μ_{s} *is norm-almost periodic;*

(ii) $\lim_{n\to\infty} \frac{|\mu_0|(A_n)}{\theta_G(A_n)} \,=\, 0.$ □

We complete this section by proving that, for weakly almost periodic measures supported inside Meyer sets, conditions (i) and (ii) in Proposition 5.8.7 characterise the weakly almost periodic decomposition due to Eberlein.

Proposition 5.8.8. *Let μ be a weakly almost periodic measure on some σ-compact LCAG G, and let $\{A_n\}$ be a van Hove sequence. Let ν_1 and ν_2 be two measures such that*

(i) $\mu = \nu_1 + \nu_2$*;*

(ii) ν_1 *is norm-almost periodic;*

(iii) $\lim_{n\to\infty} \frac{|\nu_2|(A_n)}{\theta_G(A_n)} \,=\, 0.$

Then, one has $\nu_1 = \mu_{\mathsf{s}}$ and $\nu_2 = \mu_0$.

Proof. As ν_1 is norm-almost periodic, it follows from Lemma 5.3.3 that ν_1 is strongly almost periodic. Thus, $\nu_2 = \mu - \nu_1$ is weakly almost periodic

because it is the difference of two weakly almost periodic measures. Hence, for each $f \in C_{\mathsf{c}}(G)$, the limit

$$M\big(|f * \nu_2|\big) \,=\, \lim_{n\to\infty} \frac{\int_{A_n} \big|(f * \nu_2)(s)\big| \,\mathrm{d}\theta_G(s)}{\theta_G(A_n)}$$

exists. To complete the proof, we need to show that this limit always vanishes.

Let $K := \mathrm{supp}(f)$. An easy computation shows that

$$\int_{A_n \setminus \partial^K A_n} \big|(f * \nu_2)(s)\big| \,\mathrm{d}\theta_G(s) \,\leqslant\, \big|\nu_2\big|(A_n) \int_G \big|f(s)\big| \,\mathrm{d}\theta_G(s).$$

Combining this inequality with statement (iii) and the van Hove condition, we conclude that

$$M\big(|f * \nu_2|\big) \,=\, 0.$$

Since this holds for all $f \in C_{\mathsf{c}}(G)$, it follows that ν_2 is a null-weakly almost periodic measure. The claim now follows from the uniqueness of the Eberlein decomposition of Theorem 4.10.10. □

Combining Propositions 5.8.7 and 5.8.8 provides a simple characterisation of the Eberlein decomposition of measures supported inside Meyer sets.

Corollary 5.8.9. *Let μ be a weakly almost periodic measure with Meyer set support in a σ-compact LCAG G, and let $\{A_n\}$ be a van Hove sequence. Then, μ_{s} and μ_0 are uniquely characterised by*

(i) $\mu = \mu_{\mathsf{s}} + \mu_0$;
(ii) μ_{s} *is norm-almost periodic;*
(iii) $\lim_{n\to\infty} \frac{|\mu_0|(A_n)}{\theta_G(A_n)} \,=\, 0$. □

5.9. Diffraction of weighted Dirac combs on Meyer sets

The diffraction of Meyer sets in $\mathbb{R}^d$ was studied in [43, 44]. As the two papers use two different characterisations of Meyer sets, which were known to be equivalent in $\mathbb{R}^d$ but not in general LCAGs, it was previously not clear whether (and how) these results could be generalised beyond the case $G = \mathbb{R}^d$. The characterisation given in Theorem 5.7.8 settles this problem.

Below, we use the results from Section 5.8 to study the diffraction measures of weighted Dirac combs that are supported inside Meyer sets. This generalises all the results of [43, 44] in two directions, namely from the case $G = \mathbb{R}^d$ to a general σ-compact LCAG and from Meyer sets to arbitrary complex-weighted Dirac combs that are supported inside Meyer sets. We start by recalling a lemma which we will use several times below.

Lemma 5.9.1 ([43, Prop. 3.5])**.** *Let $\mu \neq 0$ be a strongly almost periodic measure in some LCAG G. Then,* $\mathrm{supp}(\mu)$ *is relatively dense in G.* □

Now we use Corollary 5.8.2 to show that both the pure point and the continuous part of the diffraction measure of a weighted Dirac comb with Meyer set support are almost periodic measures.

Theorem 5.9.2. *Let ω be a weighted Dirac comb supported inside some Meyer set in a σ-compact LCAG G, and let γ be an autocorrelation for ω, relative to a given van Hove sequence. Then, $\widehat{\gamma}_{\mathsf{pp}}$ and $\widehat{\gamma}_{\mathsf{c}}$ are strongly almost periodic measures.*

In particular, the pure point part and the continuous part of the diffraction measure $\widehat{\gamma}$ of ω are each either trivial or have relatively dense support in the dual group $\widehat{G}$.

Proof. Let $\varLambda$ be any Meyer set containing $\operatorname{supp}(\omega)$. Then, $\operatorname{supp}(\gamma) \subseteq \varLambda - \varLambda$. It follows from Corollary 5.7.10 that $\operatorname{supp}(\gamma)$ is a subset of a Meyer set. Thus, by Corollary 5.8.2, γ_{s} and γ_0 are supported inside a Meyer set, hence they both are pure point measures.

As γ is a positive definite measure, it is Fourier transformable by Theorem 4.11.5. Then, by Theorem 4.10.12, we have

$$\widehat{\gamma_{\mathsf{s}}} = \widehat{\gamma}_{\mathsf{pp}} \quad \text{and} \quad \widehat{\gamma_0} = \widehat{\gamma}_{\mathsf{c}}.$$

Hence, by Corollary 4.11.14 or [12, Cor. 11.1], both measures $\widehat{\gamma}_{\mathsf{pp}}$ and $\widehat{\gamma}_{\mathsf{c}}$ are strongly almost periodic.

The rest of the proof follows from Lemma 5.9.1. □

The next result is an immediate consequence of Theorem 5.9.2.

Corollary 5.9.3. *Let G be a σ-compact LCAG and let $M \subseteq G$ be a Meyer set with autocorrelation γ. Then, $\widehat{\gamma}_{\mathsf{pp}}$ and $\widehat{\gamma}_{\mathsf{c}}$ are strongly almost periodic, and $\widehat{\gamma}_{\mathsf{pp}} \neq 0$.*

In particular, M has a relatively dense set of Bragg peaks.[14] *Moreover, either M is pure point diffractive or M has an additional continuous diffraction component with a relatively dense support.*

Proof. The claim $\widehat{\gamma}_{\mathsf{pp}} \neq 0$ follows immediately from the observation

$$\widehat{\gamma}(\{0\}) \geqslant \bigl(\underline{\operatorname{dens}}(M)\bigr)^2 > 0;$$

compare [AO1, Cor. 9.1] for the case $G = \mathbb{R}^d$.

The rest of the proof now follows from Theorem 5.9.2. □

One simple consequence of these results is the fact that, if a Meyer set has no singularly continuous spectrum, and if its absolutely continuous spectrum is given by some uniformly continuous bounded function f, then f is automatically an almost periodic function.

[14] See Definition 5.9.12 below.

Corollary 5.9.4. *Let ω be a weighted Dirac comb on a σ-compact LCAG G. Assume further that ω is supported inside a Meyer set and let γ be an autocorrelation of ω. Suppose that $\widehat{\gamma}_{\mathsf{sc}} = 0$ and that $\widehat{\gamma}_{\mathsf{ac}} = f\theta_G$ holds for some $f \in C_{\mathsf{u}}(\widehat{G})$. Then, f is an almost periodic function on $\widehat{G}$.*

Proof. We know that the measure $\widehat{\gamma}_{\mathsf{c}} = f\theta_G$ is strongly almost periodic. By Proposition 4.10.5, f is then an almost periodic function. □

Corollary 5.9.3 tells us that, for any[15] $f \in \mathcal{K}_2(\widehat{G})$, the sets

$$P_{\mathsf{pp}}(\varepsilon; f) := \left\{t \in \widehat{G} : \left\|T_t(f * \widehat{\gamma}_{\mathsf{pp}}) - f * \widehat{\gamma}_{\mathsf{pp}}\right\|_\infty < \varepsilon\right\}$$

and

$$P_{\mathsf{c}}(\varepsilon; f) := \left\{t \in \widehat{G} : \left\|T_t(f * \widehat{\gamma}_{\mathsf{c}}) - f * \widehat{\gamma}_{\mathsf{c}}\right\|_\infty < \varepsilon\right\}$$

are relatively dense.

As our next result, we will prove directly that these sets contain some ε-dual sets, thus providing new proofs for Corollary 5.9.3 and Theorem 5.9.2. More precisely, we prove that there exists a positive constant $C := C(f; \gamma)$ such that, for any regular model set $\varGamma$ containing $\varLambda$, we have the inclusion $(\varGamma - \varGamma)^\varepsilon \subseteq P_{\mathsf{pp}}(C\varepsilon; f) \cap P_{\mathsf{c}}(C\varepsilon; f)$.

For a finite measure ν, we denote its total variation by $\|\nu\|$, that is

$$\|\nu\| := |\nu|(G).$$

Note that this defines a norm on the space of finite measures on G.

Let us recall that, given a measure μ and a Borel set A, we say that μ is *concentrated* on A if

$$|\mu|(G \setminus A) = 0.$$

Note that this is equivalent to $\mu(E) = 0$ for all Borel sets E such that $E \cap A = \varnothing$.

Lemma 5.9.5. *Let μ be a twice Fourier transformable measure, that is concentrated on $\varDelta$. Let $f \in \mathcal{K}_2(\widehat{G})$. Then, $\|\check{f}\mu\| < \infty$ and, for all $\varepsilon > 0$ and all $\chi \in \varDelta^\varepsilon$, we have*

$$\left\|T_\chi(f * \widehat{\mu}) - f * \widehat{\mu}\right\|_\infty \leqslant \left\|\check{f}\mu\right\|\varepsilon.$$

Proof. Since $f \in \mathcal{K}_2(\widehat{G})$ and $\widehat{\mu}$ is Fourier transformable, $\check{f} \in L^1(\mu)$. Hence $\check{f}\mu$ is a finite measure, and thus

$$\left\|\check{f}\mu\right\| < \infty.$$

[15] See Definition 4.9.5 for the definition of the $\mathcal{K}_2$-space.

Now, let $\chi \in \varDelta^{\varepsilon}$ and $\psi \in \widehat{G}$. Then,

$$\begin{aligned}
\bigl|T_\chi(f * \widehat{\mu})(\psi) - (f * \widehat{\mu})(\psi)\bigr| \,&=\, \bigl|(f * \widehat{T_\chi \mu})(\psi) - (f * \widehat{\mu})(\psi)\bigr| \\
&=\, \bigl|f * (\widehat{T_\chi \mu - \mu})(\psi)\bigr| \,=\, \left| \int_G \check{f}(t)\,(\chi(t)-1)\,\psi(t)\,\mathrm{d}\mu(t) \right| \\
&\leqslant \int_G \bigl|\check{f}(t)\,(\chi(t)-1)\,\psi(t)\bigr|\,\mathrm{d}|\mu|(t) \,=\, \int_{\varDelta} \bigl|\check{f}(t)\bigr|\,\bigl|\chi(t)-1\bigr|\,\bigl|\psi(t)\bigr|\,\mathrm{d}|\mu|(t) \\
&\leqslant\, \varepsilon \int_{\varDelta} \bigl|\check{f}\bigr|(t)\,\mathrm{d}|\mu|(t) \,\leqslant\, \varepsilon \bigl\|\check{f}\mu\bigr\|,
\end{aligned}$$

which completes the argument. □

Using Lemma 5.9.5 for γ_{s} and γ_0, we obtain the following result.

Proposition 5.9.6. *Let ω be a translation bounded measure, let γ be any autocorrelation for ω, and let $\varDelta$ be any set such that both γ_{s} and γ_0 are concentrated on $\varDelta$. Let $f \in \mathcal{K}_2(\widehat{G})$. If γ is twice Fourier transformable, there exists a constant $C > 0$ which depends only on f, γ_{s} and γ_0 so that, for all $\varepsilon > 0$, we have*

$$\varDelta^{\varepsilon} \,\subseteq\, P_{\mathsf{pp}}(C\varepsilon; f) \,=\, \bigl\{t \in \widehat{G} : \bigl\|T_t(f * \widehat{\gamma}_{\mathsf{pp}}) - f * \widehat{\gamma}_{\mathsf{pp}}\bigr\|_{\infty} < \varepsilon\bigr\}$$

and

$$\varDelta^{\varepsilon} \,\subseteq\, P_{\mathsf{c}}(C\varepsilon; f) \,=\, \bigl\{t \in \widehat{G} : \bigl\|T_t(f * \widehat{\gamma}_{\mathsf{c}}) - f * \widehat{\gamma}_{\mathsf{c}}\bigr\|_{\infty} < \varepsilon\bigr\}.$$

Proof. First, let us note that, since γ is Fourier transformable, so are γ_{s} and γ_0 by Theorem 4.10.12. Moreover, as $\widehat{\gamma}$ is Fourier transformable, the measures $\widehat{\gamma}_{\mathsf{pp}}$ and $\widehat{\gamma}_{\mathsf{c}}$ are also Fourier transformable by Corollary 4.11.14. This implies that both γ_{s} and γ_0 are twice Fourier transformable.

Using

$$C \,:=\, \max\Bigl\{\bigl\|\check{f}\gamma_{\mathsf{s}}\bigr\|, \bigl\|\check{f}\gamma_0\bigr\|\Bigr\},$$

the statements on $\varDelta^{\varepsilon}$ become immediate consequences of Lemma 5.9.5. □

Note that, unless $\varDelta$ is uniformly discrete, $\varDelta^{\varepsilon}$ cannot be relatively dense. If $\varLambda$ is Meyer, combining Theorem 5.9.2 with Proposition 5.9.6 establishes the following result for the CPS $(G, H, \mathcal{L})$.

Proposition 5.9.7. *Let G be a σ-compact LCAG and let ω be a weighted Dirac comb on G that is supported inside some Meyer set. Let $\curlywedge(W)$, with $W \subseteq H$ compact, be a regular*[16] *model set containing* $\mathrm{supp}(\omega)$*, and consider $\varDelta := \curlywedge(W) - \curlywedge(W)$. Let γ be an autocorrelation of ω and fix some function $f \in \mathcal{K}_2(\widehat{G})$.*

[16]Here, the attribute 'regular' refers to the property that the boundary ∂W of the window has Haar measure 0 in H; see [30] and [AO1] for more.

If γ is twice Fourier transformable, there exists a $C > 0$ which depends only on f, γ_{s} and γ_0, such that, for all $\varepsilon > 0$, we have

$$\varDelta^{\varepsilon} \subseteq P_{\mathsf{pp}}(C\varepsilon; f) = \big\{t \in \widehat{G} : \big\|T_t(f * \widehat{\gamma}_{\mathsf{pp}}) - f * \widehat{\gamma}_{\mathsf{pp}}\big\|_{\infty} < \varepsilon\big\}$$

and

$$\varDelta^{\varepsilon} \subseteq P_{\mathsf{c}}(C\varepsilon; f) = \big\{t \in \widehat{G} : \big\|T_t(f * \widehat{\gamma}_{\mathsf{c}}) - f * \widehat{\gamma}_{\mathsf{c}}\big\|_{\infty} < \varepsilon\big\}.$$

In particular, $f * \widehat{\gamma}_{\mathsf{pp}}$ and $f * \widehat{\gamma}_{\mathsf{c}}$ are strongly almost periodic functions.

The following results show that, for Meyer sets and more generally for any measure whose autocorrelation is supported inside a Meyer set, the pure point spectrum is sup-almost periodic. Moreover, we show that, up to multiplication by some constant, the ε-dual sets of the support of the autocorrelation are subsets of the ε-sup-almost periods of the pure point spectrum.

Proposition 5.9.8. *Let γ be a measure on a σ-compact LCAG, and assume that γ is concentrated on $\varDelta$ and Fourier transformable. Then, there exists some $C > 0$ such that, for all $\varepsilon > 0$ and all $\psi \in \varDelta^{\varepsilon}$, we have*

$$\big|\widehat{\gamma}(\{\psi \mathbin{\hat{+}} \chi\}) - \widehat{\gamma}(\{\chi\})\big| \leqslant C\varepsilon$$

for all $\chi \in \widehat{G}$. In particular, we have

$$\varDelta^{\varepsilon/C} \subseteq P_{\varepsilon}^{\infty}\big(\widehat{\gamma}_{\mathsf{pp}}\big).$$

Proof. While this result is more general, the proof below is almost identical to the proofs of [44, Th. 3.1] and [46, Thm. 5.1]. We repeat it here for convenience.

As γ is translation bounded, there is a constant $C > 0$ such that

$$\limsup_{n\to\infty} \frac{|\gamma|(A_n)}{\theta_G(A_n)} < C.$$

Let $\chi \in \widehat{G}$ and $\psi \in \varDelta^{\varepsilon}$. Then, by Theorem 4.10.14 (see also [24, Cor. 5]), we have

$$\begin{aligned}
\big|\widehat{\gamma}(\{\psi \mathbin{\hat{+}} \chi\}) - \widehat{\gamma}(\{\chi\})\big| &= \lim_{n\to\infty}\left|\frac{\int_{A_n}\big(\psi(t)\chi(t) - \chi(t)\big)\,\mathrm{d}\gamma(t)}{\theta_G(A_n)}\right| \\
&\leqslant \limsup_{n\to\infty} \frac{\int_{A_n}\big|\psi(t)\chi(t) - \chi(t)\big|\,\mathrm{d}|\gamma|(t)}{\theta_G(A_n)} = \limsup_{n\to\infty} \frac{\int_{A_n}|\psi(t) - 1|\,\mathrm{d}|\gamma|(t)}{\theta_G(A_n)} \\
&= \limsup_{n\to\infty} \frac{\int_{A_n\cap\varDelta}|\psi(t) - 1|\,\mathrm{d}|\gamma|(t)}{\theta_G(A_n)} \leqslant \limsup_{n\to\infty} \frac{\int_{A_n\cap\varDelta}\varepsilon\,\mathrm{d}|\gamma|(t)}{\theta_G(A_n)} \\
&= \varepsilon \limsup_{n\to\infty} \frac{|\gamma|(A_n)}{\theta_G(A_n)} < \varepsilon C,
\end{aligned}$$

which completes the proof. □

Corollary 5.9.9. *Let G be a σ-compact LCAG. Further, let $\varLambda \subseteq G$ be a Meyer set and let $\varDelta = \varLambda - \varLambda$. Then, there exists a $C > 0$ so that, for all $\varepsilon > 0$, $\varDelta^{\varepsilon/C} \subseteq P_{\varepsilon}^{\infty}\bigl(\widehat{\gamma}_{\mathsf{pp}}\bigr)$. In particular, $\widehat{\gamma}_{\mathsf{pp}}$ is sup-almost periodic.* □

Combining Corollaries 5.9.9 and 5.4.4 yields the following result.

Corollary 5.9.10. *Let $\varLambda$ be a Meyer set in a σ-compact LCAG G and let $\varDelta = \varLambda - \varLambda$. Then, for all $0 < \varepsilon < 1$, the set $P_{\widehat{\gamma}(\{0\})\varepsilon}\bigl(\widehat{\gamma}_{\mathsf{pp}}\bigr)$ is a model set containing $\varDelta^{\varepsilon}$.* □

More generally, we obtain the following consequence.

Corollary 5.9.11. *Let μ be a translation bounded measure on an LCAG G, let γ be an autocorrelation for μ and let $\varDelta = \operatorname{supp}(\gamma)$. Then, there exists a $C > 0$ such that, for all $\varepsilon > 0$, one has $\varDelta^{\varepsilon/C} \subseteq P_{\varepsilon}^{\infty}\bigl(\widehat{\gamma}_{\mathsf{pp}}\bigr)$. In particular, if G is a σ-compact LCAG and if $\varDelta$ is a Meyer set in G, then the measure $\widehat{\gamma}_{\mathsf{pp}}$ is sup-almost periodic.* □

In the remainder of this section, we will study the set of positions of Bragg peaks of the diffraction measure with intensity above a certain threshold. Most of the results will hold more generally for (positive and) positive definite measures.

Definition 5.9.12. For an arbitrary positive definite measure γ on G and $a > 0$, we define

$$\mathcal{I}(a) \,:=\, \bigl\{\chi \in \widehat{G} : \widehat{\gamma}(\{\chi\}) \geqslant a\bigr\}.$$

We will call $\mathcal{I}(a)$ the set of *a-visible Bragg peak positions*, or *a-visible Bragg peaks*[17] for short.

Let $a_{\max} := \sup_{\chi\in\widehat{G}}\bigl\{\widehat{\gamma}(\{\chi\})\bigr\} = \bigl\|\widehat{\gamma}_{\mathsf{pp}}\bigr\|_{\infty}$. If γ is a positive measure, $\widehat{\gamma}$ is positive definite, and it is easy to see that $a_{\max} = I(0) = \widehat{\gamma}(\{0\})$; compare [AO1, Sec. 9.1] for the case $G = \mathbb{R}^d$.

For $a \leqslant 0$, we have $\mathcal{I}(a) = \widehat{G}$, while we have $\mathcal{I}(a) = \varnothing$ for $a > a_{\max}$. Further, Lemma 5.9.14 below shows that in general, for any non-periodic positive γ, we have $\mathcal{I}(a_{\max}) = \{0\}$. Hence, we are usually interested in the case $0 < a < a_{\max}$.

We begin by showing that, given any positive definite measure μ, we can use Krein's inequality (compare Eq. (4.3.2) or [9, Eq. (I.3.4)]) for its pure point component. The following result can also be viewed as a generalisation of [AO1, Lemma 8.4].

[17] Note that, in general, a Bragg peak is understood as a pair $(\chi, I(\chi))$ which carries the intensity information as well as the location. Here and below, we are mainly interested in the set of positions, but nevertheless we shall, by slight abuse of language, speak of Bragg peaks whenever the meaning is clear.

Lemma 5.9.13 ([27])**.** *Let μ be a positive definite measure on G. Then, the pure point part μ_{pp} of μ is a positive definite measure on G as well. Moreover, the function $f\colon G \longrightarrow \mathbb{C}$ defined by $x \mapsto f(x) = \mu(\{x\})$ is a positive definite function. In particular, for all $x, t \in G$, we have*

$$\bigl|\mu(\{x+t\}) - \mu(\{x\})\bigr|^2 \leqslant 2\mu(\{0\})\bigl[\mu(\{0\}) - \mathrm{Re}\bigl(\mu(\{t\})\bigr)\bigr].$$

Proof. For convenience, we include the proof from [27].

Since μ is positive definite, μ_{pp} is positive definite by [12, Thm. 10.2]. Thus, μ_{pp} is a positive definite pure point measure, whence it follows from [12, Thm. 10.1] that μ_{pp} is a positive definite measure on G_{d} (where G_{d} refers to G with the discrete topology). Hence, for any $g \in C_{\mathsf{c}}(G_{\mathsf{d}})$, the function $\mu_{\mathsf{pp}} * g * \widetilde{g}$ is a positive definite function on G_{d}.

Let $g := 1_{\{0\}}$ be the indicator function of the singleton set $\{0\}$. Then, $g \in C_{\mathsf{c}}(G_{\mathsf{d}})$ and

$$\bigl(\mu_{\mathsf{pp}} * g * \widetilde{g}\bigr)(x) \;=\; f(x).$$

Hence, f is a positive definite function on G_{d}; compare Definition 4.3.7. It follows immediately that f is also positive definite on G, since, for all $n \in \mathbb{N}$ and all $x_1, \ldots, x_n \in G$, the matrix $\bigl(f(x_i - x_j)\bigr)_{1 \leqslant i,j \leqslant n}$ is positive Hermitian.

The last claim is a reformulation of Krein's inequality for the function f via $f(x) = \mu(\{x\})$. □

Lemma 5.9.14. *Let γ be a positive and positive definite measure. If one has $\widehat{\gamma}(\{\chi\}) = a_{\max}$ for some non-trivial χ, then χ is a period for $\widehat{\gamma}$.*

Proof. Since $\widehat{\gamma}$ is a positive definite measure, Lemma 5.9.13 implies that the inequality

$$\bigl|\widehat{\gamma}(\{\chi \mathbin{\hat{+}} \psi\}) - \widehat{\gamma}(\{\psi\})\bigr|^2 \leqslant 2\,\widehat{\gamma}(\{0\})\,\bigl[\widehat{\gamma}(\{0\}) - \mathrm{Re}\bigl(\widehat{\gamma}(\{\chi\})\bigr)\bigr]$$

holds for all $\psi \in \widehat{G}$. Since $\widehat{\gamma}(\{0\}) = a_{\max} = \widehat{\gamma}(\{\chi\}) \in [0, \infty)$, we conclude that

$$\bigl|\widehat{\gamma}(\{\chi \mathbin{\hat{+}} \psi\}) - \widehat{\gamma}(\{\psi\})\bigr|^2 \leqslant 0,$$

which completes the proof. □

Next, we extend [44, Thm. 4.4] to an arbitrary LCAG.

Corollary 5.9.15. *Let γ be a positive definite measure on a σ-compact LCAG G, with $\widehat{\gamma}_{\mathsf{pp}} \neq 0$ and $\varDelta = \mathrm{supp}(\gamma)$. If $\varDelta$ is a Meyer set, then, for all $0 < a < a_{\max}$, the set of a-visible Bragg peaks is a Meyer set.*

Proof. Pick some $C > 0$ as in Proposition 5.9.8. Let $0 < a < a_{\max}$ and fix some $0 < \varepsilon < \max\bigl\{\frac{a_{\max}-a}{C}, \frac{a}{C}, \frac{\sqrt{3}}{2}\bigr\}$.

We first show that $\mathcal{I}(a)$ contains a translate of $\varDelta^{\varepsilon}$. As $a + C\varepsilon < a_{\max}$, the definition of $a_{\max}$ implies the existence of some ϕ such that

$$\widehat{\gamma}(\{\phi\}) \, > \, a + C\varepsilon .$$

Let $\psi \in \varDelta^{\varepsilon}$ be arbitrary. By Proposition 5.9.8, we have

$$\bigl|\widehat{\gamma}(\{\psi \mathbin{\hat{+}} \phi\}) - \widehat{\gamma}(\{\phi\})\bigr| \, \leqslant \, C\varepsilon \, < \, \widehat{\gamma}(\{\phi\}) - a .$$

Hence $\widehat{\gamma}(\{\psi \mathbin{\hat{+}} \phi\}) \geqslant a$, and thus

$$\phi \mathbin{\hat{+}} \varDelta^{\varepsilon} \, \subseteq \, \mathcal{I}(a).$$

Next, we show that $\mathcal{I}(a)$ is contained in finitely many translates of $\varDelta^{\varepsilon}$. By Proposition 5.9.8, for all $\psi \in \varDelta^{\varepsilon}$ and $\chi \in \mathcal{I}(a)$, we have

$$\bigl|\widehat{\gamma}(\{\psi \mathbin{\hat{\pm}} \chi\}) - \widehat{\gamma}(\{\chi\})\bigr| \, \leqslant \, C\varepsilon .$$

Thus

$$\widehat{\gamma}(\{\psi \mathbin{\hat{\pm}} \chi\}) \, \geqslant \, a - C\varepsilon \, > \, 0$$

and

$$\mathcal{I}(a) \mathbin{\hat{\pm}} \varDelta^{\varepsilon} \, \subseteq \, \mathcal{I}(a - C\varepsilon).$$

Since $\varDelta$ is a Meyer set and $\varepsilon < \frac{\sqrt{3}}{2}$, the set $\varDelta^{\varepsilon}$ is relatively dense. So, there exists a compact set $K \subseteq \widehat{G}$ with $\varDelta^{\varepsilon} \mathbin{\hat{+}} K = \widehat{G}$. Since $\widehat{\gamma}$ is translation bounded and $a - C\varepsilon > 0$, the set $\mathcal{I}(a - C\varepsilon)$ is locally finite. Consequently, $F := \mathcal{I}(a - C\varepsilon) \cap K$ is a finite set.

Now, let $\chi \in \mathcal{I}(a)$ be arbitrary. Then $\chi \in G$, hence $\chi = \psi \mathbin{\hat{+}} \varphi$ with $\psi \in \varDelta^{\varepsilon}$ and $\varphi \in K$. Consequently,

$$\varphi \, = \, \chi \mathbin{\hat{-}} \psi \, \in \, \mathcal{I}(a) \mathbin{\hat{-}} \varDelta^{\varepsilon} \, \subseteq \, \mathcal{I}(a - C\varepsilon),$$

and hence $\varphi \in F$. This proves that $\mathcal{I}(a) \subseteq \varDelta^{\varepsilon} \mathbin{\hat{+}} F$. Since $\varLambda$ is a Meyer set, so is $\varDelta$ and hence, by Theorem 5.7.8, $\varDelta^{\varepsilon}$ is a Meyer set. Therefore, $\varDelta^{\varepsilon} \mathbin{\hat{+}} F$ is a Meyer set, and because

$$\phi \mathbin{\hat{+}} \varDelta^{\varepsilon} \, \subseteq \, \mathcal{I}(a) \, \subseteq \, \varDelta^{\varepsilon} \mathbin{\hat{+}} F,$$

we conclude that $\mathcal{I}(a)$ is a Meyer set as well. □

Corollary 5.9.16. *Let $\varLambda$ be a Meyer set in a σ-compact LCAG G. Then, for all $0 < a < \widehat{\gamma}(\{0\})$, the set of a-visible Bragg peaks is a Meyer set.* □

Note that all results in this section depend on the autocorrelation we may choose for the Meyer set. In general, a Meyer set can have several distinct autocorrelations. We will conclude this section by addressing an interesting question posed by Michael Baake, namely, given two different autocorrelations of the same Meyer set, how different can the two diffractions be? As we shall see, there is little if any connection between their continuous components, while their pure point parts do show a structural relation.

Example 5.9.17. Let $\varLambda_1, \varLambda_2 \subseteq \mathbb{R}$ be two Meyer subsets of the same model set. Let

$$\varLambda \, := \, \big[\varLambda_1 \cap (-\infty, 0)\big] \cup \big[\varLambda_2 \cap [0, \infty)\big] .$$

If $A_n = (-n^2, n)$ or $A_n = (-n^2, 0)$, then any autocorrelation of $\varLambda$ with respect to A_n is actually an autocorrelation of $\varLambda_1$. Similarly, if $B_n = (-n, n^2)$ or $B_n = (0, n)$, then any autocorrelation of $\varLambda$ with respect to B_n is actually an autocorrelation of $\varLambda_2$.

Now, let $\varLambda_1 = \mathbb{Z}$ and $\varLambda_2 = 2\mathbb{Z} \cup S$ where S is a typical Bernoulli subset of $2\mathbb{Z} + 1$ (with occupation probability $p = \frac{1}{2}$ to be specific). Note that $\varLambda_2$ is always a Meyer set; see [AO1, Ex. 2.4]. If we now choose a van Hove sequence $(C_m)_{m \in \mathbb{N}}$ via $C_{2n} = [0, n^2]$ and $C_{2n+1} = [-n^2, 0]$, the Meyer set $\varLambda := \big[\varLambda_1 \cap (-\infty, 0)\big] \cup \big[\varLambda_2 \cap [0, \infty)\big]$ has both

$$\gamma_1 \, = \, \delta_{\mathbb{Z}} \quad \text{and} \quad \gamma_2 \, = \, \frac{5}{8}\delta_{2\mathbb{Z}} + \frac{1}{2}\delta_{2\mathbb{Z}+1} + \frac{1}{8}\delta_0$$

as autocorrelations, where the second follows from a standard application of the strong law of large numbers; compare [AO1, Sec. 11.2]. While γ_1 leads to a pure point diffraction measure, γ_2 produces a mixed (pure point and absolutely continuous) measure, namely

$$\widehat{\gamma_2} \, = \, \frac{9}{16}\delta_{\mathbb{Z}} + \frac{1}{16}\delta_{\mathbb{Z}+\frac{1}{2}} + \frac{1}{8}\lambda,$$

where λ denotes Lebesgue measure.

Let us now set $\varLambda_1 = \mathbb{Z}$ and choose $\varLambda_3$ as the set of a-type positions of the Thue–Morse chain; compare [AO1, Sec. 4.6] for the setting. If we now consider $\varLambda := \big[\varLambda_1 \cap (-\infty, 0)\big] \cup \big[\varLambda_3 \cap [0, \infty)\big]$, then, with respect to the van Hove sequence (C_m) from above, $\varLambda$ possesses two different autocorrelations. One of these corresponds to a pure point diffraction, and the other to a mixed (pure point and singular continuous) diffraction.

One can also mix the Thue–Morse system with a Bernoulli system such as $\varLambda_2$ from above to construct a Meyer set with different autocorrelations. In this case, the corresponding diffraction measures are mixed, with one being pure point and absolutely continuous, the other pure point and singular continuous. $\diamondsuit$

While the systems of Example 5.9.17 are not homogeneous, they are natural in the following sense. If $\varLambda$ has two different autocorrelation measures, it means that there are arbitrarily large finite parts of $\varLambda$ that have different statistical properties, and thus are significantly different. In the above examples, the two 'halves' (parts) of $\varLambda$ are completely different by construction. A more interesting system is the following one.

Example 5.9.18. As in Example 5.9.17, consider $\varLambda_1 = \mathbb{Z}$, $\varLambda_2$ a typical Bernoulli Meyer system, and $\varLambda_3$ the a-type Thue–Morse set. Let

$$\varLambda := \left[\bigcup_{n\in\mathbb{N}} \left[\varLambda_1 \cap \pm\left[3^{3n}, 3^{3n+1}\right)\right]\right] \cup \left[\bigcup_{n\in\mathbb{N}} \left[\varLambda_2 \cap \pm\left[3^{3n+1}, 3^{3n+2}\right)\right]\right] \cup \left[\bigcup_{n\in\mathbb{N}} \left[\varLambda_3 \cap \pm\left[3^{3n+2}, 3^{3n+3}\right)\right]\right].$$

Then, $\varLambda$ has the autocorrelations of each of $\varLambda_1$, $\varLambda_2$ and $\varLambda_3$ as cluster points, as well as various convex combinations of these autocorrelations. ◊

This example shows that, given two different autocorrelations of the same Meyer set, we should not expect any connection between their continuous diffraction measures. But what about the pure point diffraction spectra?

Let $\varLambda$ be a Meyer set and let γ_1 and γ_2 be two autocorrelations of $\varLambda$. Let $\varGamma$ be any regular model set containing $\varLambda$. Then, as we saw in the proof of Theorem 5.9.2, since the autocorrelation γ of $\varGamma$ exists and is independent of the choice of van Hove sequence, there exist some finite sets F_1 and F_2 such that

$$(\gamma_1)_{\mathsf{s}} \leqslant \gamma \leqslant \delta_{F_1} * (\gamma_1)_{\mathsf{s}} \quad \text{and} \quad (\gamma_2)_{\mathsf{s}} \leqslant \gamma \leqslant \delta_{F_2} * (\gamma_2)_{\mathsf{s}}.$$

Combining these two relations, we obtain

$$(\gamma_1)_{\mathsf{s}} \leqslant \delta_{F_2} * (\gamma_2)_{\mathsf{s}} \quad \text{and} \quad (\gamma_2)_{\mathsf{s}} \leqslant \delta_{F_1} * (\gamma_1)_{\mathsf{s}}.$$

Thus, we see that the strongly almost periodic components of the two autocorrelations are certainly related. However, it is not obvious how restrictive these inequalities really are.

By combining the results in this section with Theorem 5.7.8, we get the following general characterisation.

Theorem 5.9.19. *Let $\varLambda \subseteq G$ be relatively dense, where G is a σ-compact LCAG. Then, the following statements are equivalent.*

(i) *$\varLambda$ is a subset of a model set.*

(ii) *$\varLambda^{\varepsilon}$ is relatively dense for all $0 < \varepsilon < 2$.*

(iii) *$\varLambda^{\varepsilon}$ is a model set for all $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(iv) *$\varLambda^{\varepsilon}$ is a model set for some $0 < \varepsilon < \frac{\sqrt{3}}{2}$.*

(v) *$\varLambda^{\varepsilon}$ is relatively dense for some $0 < \varepsilon < \frac{\sqrt{3}}{6}$.*

(vi) *$\varLambda$ is an almost lattice.*

(vii) *$\varLambda - \varLambda - \varLambda$ is locally finite.*

(viii) *There exists a sup-almost periodic, pure point Radon measure η and an $0 < \varepsilon < \|\eta\|_{\infty}$ such that $\varLambda \subseteq P_{\varepsilon}^{\infty}(\eta)$.*

(ix) *There exists a strongly almost periodic measure* η *on* G*, with the set* $\operatorname{supp}(\eta) - \operatorname{supp}(\eta)$ *being uniformly discrete, such that* $\varLambda \subseteq \operatorname{supp}(\eta)$.

(x) *There exists a sup-almost periodic, pure point Radon measure* η *such that* $\operatorname{supp}(\eta)$ *has finite local complexity and* $\varLambda \subseteq \operatorname{supp}(\eta)$.

(xi) *There exists a norm-almost periodic pure point measure* η *such that* $\operatorname{supp}(\eta)$ *has finite local complexity and* $\varLambda \subseteq \operatorname{supp}(\eta)$.

(xii) *There exists a sup-almost periodic Radon measure* η *together with a constant* $a > 0$ *such that* $\operatorname{supp}(\eta)$ *has finite local complexity and that* $\varLambda \subseteq \{x \in G : |\eta(\{x\})| > a\}$.

(xiii) *There exists a sup-almost periodic Radon measure* η *such that its support* $\operatorname{supp}(\eta)$ *has finite local complexity and* $\delta_{\varLambda} \leqslant \eta$.

(xiv) *There exists a norm-almost periodic measure* η *such that* $\operatorname{supp}(\eta)$ *has finite local complexity and* $\delta_{\varLambda} \leqslant \eta$.

PROOF. We already know that the first seven conditions are equivalent. Since any norm-almost periodic measure is sup-almost periodic, the implication (xiv) $\Longrightarrow$ (xiii) is obvious. Also, by picking any $0 < a < 1$, the implication (xiii) $\Longrightarrow$ (xii) is trivial, while (xii) $\Longrightarrow$ (x) is immediate. Furthermore, (ix) $\Longleftrightarrow$ (x) $\Longleftrightarrow$ (xi) $\Longrightarrow$ (i) follows from Theorem 5.5.2, and (viii) $\Longrightarrow$ (i) from Corollary 5.4.4.

We now show that (i) $\Longrightarrow$ (viii). Pick $0 < \varepsilon < \frac{1}{2}$. Then, $\varLambda^{\varepsilon}$ is a model set. Let γ be the autocorrelation of $\varLambda^{\varepsilon}$ and let $\varGamma := \varLambda^{\varepsilon} \mathbin{\tilde{-}} \varLambda^{\varepsilon}$. Since $0 \in \varLambda^{\varepsilon}$, we have that $\varLambda^{\varepsilon} \subseteq \varGamma$. By Proposition 5.9.8, for all $x \in G$, $\varepsilon' > 0$ and $y \in \varGamma^{\varepsilon'}$, we have

$$\left|\widehat{\gamma}(\{x+y\}) - \widehat{\gamma}(\{x\})\right| \leqslant \widehat{\gamma}(\{0\})\varepsilon'.$$

Thus, for all $\varepsilon' < 1$, we obtain $\widehat{\gamma}(\{0\})\varepsilon' < \|\widehat{\gamma}_{\mathsf{pp}}\|_{\infty} = \widehat{\gamma}(\{0\})$ and

$$\varGamma^{\varepsilon'} \subseteq P_{\widehat{\gamma}(\{0\})\varepsilon'}\big(\widehat{\gamma}_{\mathsf{pp}}\big).$$

Thus, $\widehat{\gamma}_{\mathsf{pp}}$ is sup-almost periodic. Also, by Lemma 5.6.9, we have

$$(\varLambda^{\varepsilon})^{\varepsilon} \subseteq \varGamma^{2\varepsilon}.$$

Since $2\varepsilon < 1$, we thus obtain

$$\varLambda \subseteq (\varLambda^{\varepsilon})^{\varepsilon} \subseteq \varGamma^{2\varepsilon} \subseteq P_{2\widehat{\gamma}(\{0\})\varepsilon}\big(\widehat{\gamma}_{\mathsf{pp}}\big).$$

As $\widehat{\gamma}_{\mathsf{pp}}$ is sup-almost periodic, we are done.

To complete the proof, we show that (i) $\Longrightarrow$ (xiv) by constructing a measure that satisfies (xiv). Our measure will also satisfy the condition (xi), but this implication is not needed.

Let $(G, H, \mathcal{L})$ be a CPS and let $W \subseteq H$ be a compact set such that $\varLambda \subseteq \curlywedge(W)$. Let $g \in C_{\mathsf{c}}(H)$ be such that $g \geqslant 1_W$, and let $\eta := \omega_g$. Since $\operatorname{supp}(\eta)$ is a model set and $\|g\|_{\infty} < \infty$, it is easy to see that η is a Radon

measure. Moreover, $\delta_{\varLambda} \leqslant \eta$. Then, by Theorem 5.5.2, the measure η is sup-almost periodic. As a model set, $\operatorname{supp}(\eta)$ has finite local complexity. Moreover,

$$\varLambda \subseteq \left\{ x \in G : \eta(\{x\}) > \tfrac{1}{2} \right\} \subseteq \operatorname{supp}(\eta),$$

which completes the argument. □

As an immediate consequence of this result we obtain that every Meyer set is a subset of a model set with metrisable and compactly generated internal space.

Corollary 5.9.20. *Let $\varLambda$ be a Meyer set in a σ-compact LCAG G. Then, there exists a CPS $(G, H, \mathcal{L})$ with H a metrisable and compactly generated LCAG, and a compact set $W \subseteq H$ such that*

$$\varLambda = \curlywedge(W).$$

Proof. By Theorem 5.9.19, there exists a strongly almost periodic measure ω on G, with the set $\operatorname{supp}(\omega) - \operatorname{supp}(\omega)$ being uniformly discrete, such that $\varLambda \subseteq \operatorname{supp}(\omega)$.

Next, by Theorem 5.5.2, there exists a CPS $(G, H, \mathcal{L})$ with H compactly generated and metrisable together with a function $f \in C_{\mathsf{c}}(H)$ so that

$$\omega \,=\, \omega_f \,= \sum_{x \in L} f(x^{\star})\, \delta_x .$$

The claim now follows by choosing $W := \operatorname{supp}(f)$. □

Given a Meyer set $\varLambda$ with autocorrelation γ, we proved earlier that the set $\mathcal{I}(a)$ of a-visible Bragg peaks in the diffraction measure of $\varLambda$ is a Meyer set for all $0 < a < \widehat{\gamma}(\{0\})$. In the remainder of this section, we extend this result to any measure μ with positive autocorrelation measure γ and relatively dense sets of a-visible Bragg peaks. One particularly interesting example which satisfies this condition is the set of visible lattice points [8, 15, 3, 34]; see also [AO1, Sec. 10.4].

In $\mathbb{R}^d$, given a measure μ with positive autocorrelation γ, it was shown in [27] that, if the set of a-visible Bragg peaks is relatively dense for some a with $\widehat{\gamma}(\{0\}) \left(\sqrt{3} - 1\right) < a < \widehat{\gamma}(\{0\})$, then it must be a Meyer set.

We start by proving that if all the sets of a-visible Bragg peaks are relatively dense, then they are model sets in the same CPS. In particular, this is the case for the diffraction of a Meyer set. We then prove a result similar to the one in [27] for a single set of a-visible Bragg peaks, with a large enough.

Proposition 5.9.21. *Let μ be a measure and let γ be an autocorrelation of μ. If γ is positive and $\widehat{\gamma}(\{0\}) > 0$, the following statements are equivalent.*

(i) *For every* $0 < a < \widehat{\gamma}(\{0\})$*, the set* $\mathcal{I}(a)$ *of* a*-visible Bragg peaks is relatively dense.*

(ii) *For all* $0 < a < \widehat{\gamma}(\{0\})$*, the sets* $\mathcal{I}(a)$ *of* a*-visible Bragg peaks are model sets in the same CPS.*

(iii) *There exists a CPS*[18] $(\widehat{G}, H_{\mathsf{fd}}, \mathcal{L}_{\mathsf{fd}})$ *together with a continuous function* $g_{\mathsf{fd}} \in C_0(H_{\mathsf{fd}})$ *so that* $\widehat{\gamma}_{\mathsf{pp}} = \omega_{g_{\mathsf{fd}}}$.

Proof. The implication (ii) $\Longrightarrow$ (i) is obvious.

We now prove (i) $\Longrightarrow$ (iii). Let $0 < \varepsilon < \sqrt{2}\,\widehat{\gamma}(\{0\})$, let $\psi \in \widehat{G}$ and choose some $\chi \in \mathcal{I}\bigl(\widehat{\gamma}(\{0\}) - \frac{\varepsilon^2}{2\widehat{\gamma}(\{0\})}\bigr)$. Then, by Lemma 5.9.13, we have

$$\bigl|\widehat{\gamma}(\psi \mathbin{\hat{+}} \chi) - \widehat{\gamma}(\psi)\bigr|^2 \,<\, 2\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - \widehat{\gamma}(\{\chi\})\bigr] \,<\, \varepsilon^2,$$

hence

$$\mathcal{I}\biggl(\widehat{\gamma}(\{0\}) - \frac{\varepsilon^2}{2\,\widehat{\gamma}(\{0\})}\biggr) \,\subseteq\, P_{\varepsilon}^{\infty}\bigl(\widehat{\gamma}_{\mathsf{pp}}\bigr).$$

As $\mathcal{I}\bigl(\widehat{\gamma}(\{0\}) - \frac{\varepsilon^2}{2\,\widehat{\gamma}(\{0\})}\bigr)$ is relatively dense, so is $P_{\varepsilon}^{\infty}\bigl(\widehat{\gamma}_{\mathsf{pp}}\bigr)$. This proves that $\widehat{\gamma}_{\mathsf{pp}}$ is a sup-almost periodic pure point measure. The conclusion now follows from Theorem 5.4.2.

We next prove (iii) $\Longrightarrow$ (ii). Since γ is positive and positive definite, we have $\widehat{\gamma}(\{0\}) \geqslant |\widehat{\gamma}(\{\chi\})| = \widehat{\gamma}(\{\chi\})$ for all $\chi \in \widehat{G}$. As $0 \leqslant g_{\mathsf{fd}}(\chi^\star) \leqslant g_{\mathsf{fd}}(0)$ for all $(\chi, \chi^\star) \in \mathcal{L}_{\mathsf{fd}}$, and since $\pi_2\bigl(\mathcal{L}_{\mathsf{fd}}\bigr)$ is dense in H_{fd}, it follows immediately from the continuity of g_{fd} that $g_{\mathsf{fd}} \geqslant 0$ and that $\|g_{\mathsf{fd}}\|_\infty = g_{\mathsf{fd}}(0) = \widehat{\gamma}(\{0\})$.

Let $0 < a < \widehat{\gamma}(\{0\}) = g_{\mathsf{fd}}(0)$ and $W_a := \{y \in H_{\mathsf{fd}} : g_{\mathsf{fd}}(y) \geqslant a\}$. Since $g_{\mathsf{fd}} \in C_0(H_{\mathsf{fd}})$, the set W_a is compact. Moreover, since $a < g_{\mathsf{fd}}(0)$, the set $W_a \subseteq H_{\mathsf{fd}}$ contains the non-empty open set $\{y \in H_{\mathsf{fd}} : g_{\mathsf{fd}}(y) > a\}$. Therefore, W_a is a compact set with non-empty interior. As $\widehat{\gamma}_{\mathsf{pp}} = \omega_{g_{\mathsf{fd}}}$, it follows from the general definition of a Dirac comb of the form ω_g that

$$\bigl\{\chi \in \widehat{G} : \widehat{\gamma}(\{\chi\}) \neq 0\bigr\} \,\subseteq\, \pi_1\bigl(\mathcal{L}_{\mathsf{fd}}\bigr).$$

Consequently,

$$\mathcal{I}(a) \,=\, \bigl\{\chi \in \widehat{G} : \widehat{\gamma}(\{\chi\}) \geqslant a\bigr\} \,=\, \bigl\{\chi : (\chi, \chi^\star) \in \mathcal{L}_{\mathsf{fd}},\, g_{\mathsf{fd}}(\chi^\star) \geqslant a\bigr\} \,=\, \curlywedge(W_a),$$

which completes the proof. □

Now, let us look at a single $\mathcal{I}(a)$. Our goal is to prove that, if a is close enough to $\widehat{\gamma}(\{0\})$, then $\mathcal{I}(a)$ is a Meyer set. Our proofs below extend the proofs of [27] from $G = \mathbb{R}^d$ to G a general LCAG that is σ-compact (which is implicitly assumed below). The key to the proof is Lemma 5.9.22 below, which shows that, if χ and ψ are Bragg peaks of high intensity, then $\chi \mathbin{\hat{+}} \psi$

[18] For later convenience, we use the index fd to denote objects that emerge via some sort of Fourier duality.

is also a Bragg peak whose intensity is bounded from below by a quantity which only depends on the intensities of the Bragg peaks at χ and ψ.

Lemma 5.9.22. *Let μ be a measure with positive autocorrelation γ. Let $0 < a, b < \widehat{\gamma}(\{0\})$. Then,*

$$\mathcal{I}(a) \mathbin{\hat{\pm}} \mathcal{I}(b) \subseteq \mathcal{I}\Bigl(b - \sqrt{2\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - a\bigr]}\,\Bigr).$$

Proof. Let $\chi \in \mathcal{I}(a)$ and $\psi \in \mathcal{I}(b)$. Then, as $\widehat{\gamma}$ is positive and positive definite, Lemma 5.9.13 implies that

$$\bigl|\widehat{\gamma}(\{\psi \mathbin{\hat{\pm}} \chi\}) - \widehat{\gamma}(\{\psi\})\bigr|^2 \leqslant 2\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - \widehat{\gamma}(\{\chi\})\bigr]$$

and hence

$$\begin{aligned}\widehat{\gamma}(\{\psi \mathbin{\hat{\pm}} \chi\}) &\geqslant b - \sqrt{2\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - \widehat{\gamma}(\{\chi\})\bigr]}\\ &\geqslant b - \sqrt{2\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - a\bigr]},\end{aligned}$$

which completes the argument. □

A simple induction on n combined with Lemma 5.9.22 yields the following result.

Corollary 5.9.23. *Let μ be a measure with positive autocorrelation γ and let $0 < a < \widehat{\gamma}(\{0\})$. Then,*

$$\underbrace{\mathcal{I}(a) \mathbin{\hat{\pm}} \mathcal{I}(a) \mathbin{\hat{\pm}} \ldots \mathbin{\hat{\pm}} \mathcal{I}(a)}_{n \text{ terms}} \subseteq \mathcal{I}\Bigl(a - (n-1)\sqrt{2\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - a\bigr]}\,\Bigr). \qquad \square$$

We are now ready to prove that, if $\mathcal{I}(a)$ is relatively dense for some a close enough to $\widehat{\gamma}(\{0\})$, then $\mathcal{I}(a)$ is a Meyer set.

Proposition 5.9.24. *Let μ be a measure with positive autocorrelation γ. Let $\widehat{\gamma}(\{0\})\bigl(\sqrt{24} - 4\bigr) < a < \widehat{\gamma}(\{0\})$. If the set $\mathcal{I}(a)$ of a-visible Bragg peaks is relatively dense, then $\mathcal{I}(a)$ is a Meyer set.*

Proof. We start by observing that

$$\begin{aligned}0 &< a - 2\sqrt{2\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - a\bigr]} &&\iff\\ a^2 &> 8\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - a\bigr] &&\iff\\ 24\bigl(\widehat{\gamma}(\{0\})\bigr)^2 &< a^2 + 8\,\widehat{\gamma}(\{0\})\,a + 16\bigl(\widehat{\gamma}(\{0\})\bigr)^2 &&\iff\\ 24\bigl(\widehat{\gamma}(\{0\})\bigr)^2 &< \bigl[a + 4\widehat{\gamma}(\{0\})\bigr]^2 &&\iff\\ a &> \widehat{\gamma}(\{0\})\bigl(\sqrt{24} - 4\bigr).\end{aligned}$$

Therefore, our hypothesis implies that $a - 2\sqrt{2\,\widehat{\gamma}(\{0\})\bigl[\widehat{\gamma}(\{0\}) - a\bigr]} > 0$.

As $\widehat{\gamma}$ is a translation bounded measure, the set $\mathcal{I}(b)$ must be locally finite for all $b > 0$. In particular, $\mathcal{I}\Big(a - 2\sqrt{2\,\widehat{\gamma}(\{0\})\big[\widehat{\gamma}(\{0\}) - a\big]}\,\Big)$ is locally finite. By Corollary 5.9.23, we have

$$\mathcal{I}(a) \mathbin{\hat{\pm}} \mathcal{I}(a) \mathbin{\hat{\pm}} \mathcal{I}(a) \subseteq \mathcal{I}\Big(a - 2\sqrt{2\,\widehat{\gamma}(\{0\})\big[\widehat{\gamma}(\{0\}) - a\big]}\,\Big).$$

Therefore, $\mathcal{I}(a) \mathbin{\hat{-}} \mathcal{I}(a) \mathbin{\hat{-}} \mathcal{I}(a)$ is a locally finite set, which proves our claim. □

We complete this section by showing that any point set having relatively dense sets of visible Bragg peak positions shares many of them with a regular model set.

Proposition 5.9.25. *Let $\varLambda$ be a Delone set, and let γ be an autocorrelation of $\varLambda$. If, for all $0 < a < \widehat{\gamma}(\{0\})$, the set $\mathcal{I}(a)$ of visible Bragg peaks is relatively dense, then there exists a regular model set $\varLambda'$ such that*

(i) *$\varLambda$ and $\varLambda'$ share a relative dense set of Bragg peak positions;*

(ii) *the sets of visible Bragg peak positions of $\varLambda$ and $\varLambda'$ are equivalent by finite translations, that is, each set can be covered by finitely many translates of the other set.*

Proof. By Proposition 5.9.21, the set of a-visible Bragg peaks $\mathcal{I}_{\varLambda}(a)$ of $\varLambda$ is a model set for all $0 < a < \widehat{\gamma}(\{0\})$. Pick some $0 < \varepsilon < \frac{\sqrt{3}}{4}$ and some $0 < a < \widehat{\gamma}(\{0\})$ such that $\widehat{\gamma}(\{0\}) - a < \varepsilon$. For the remainder of the proof, a and ε are fixed.

Observe that $\varLambda'' := \mathcal{I}_{\varLambda}(a)^{\varepsilon}$ is a model set. We next prove that there exists a regular model set $\varLambda'$ contained in $\varLambda''$. Let $(G, H, \mathcal{L})$ be a CPS and $W \subseteq H$ be a window which gives $\varLambda''$. Since W has non-empty interior, we can pick a non-trivial $h \in C_{\mathsf{c}}(H)$ such that $\operatorname{supp}(h) \subseteq W$. Then, by Theorem 5.5.2, there exists a CPS $(G, H', \mathcal{L}')$ with H' metrisable and some function $h' \in C_{\mathsf{c}}(H')$ such that

$$\omega_h = \omega_{h'}.$$

Now, since h is non-trivial, it follows that h' is non-trivial as well. Therefore, we can find some open sets $V \subseteq U \subseteq H'$ such that $h'(x) \neq 0$ for all $x \in U$ and $\overline{V} \subseteq U$. Since $U \subseteq \operatorname{supp}(h')$, which is compact, it follows that $\overline{V}$ is compact in H'.

Therefore, by [16, Lemma 3.6], there exists a compact set $\overline{V} \subseteq K \subseteq U$ with boundary measure zero. Defining

$$\varLambda' := \curlywedge(K),$$

in the CPS $(G, H', \mathcal{L}')$ gives us a regular model set $\varLambda'$. Now, by construction we have

$$\varLambda' \subseteq \operatorname{supp}(\omega_{h'}) = \operatorname{supp}(\omega_h) \subseteq \varLambda''.$$

We prove that $\varLambda'$ has the desired properties. We start by proving (i). Let η be any autocorrelation of $\varLambda'$. As $\operatorname{supp}(\eta) \subseteq \varLambda' - \varLambda'$, for all $\varepsilon' > 0$ and all $\psi \in (\varLambda' - \varLambda')^{\varepsilon'}$, Theorem 5.9.8 implies

$$\bigl|\widehat{\eta}(\{\psi\}) - \widehat{\eta}(\{0\})\bigr| \leqslant \widehat{\eta}(\{0\})\,\varepsilon'.$$

Thus, for all $0 < \varepsilon' < 1$, we obtain

$$\widehat{\eta}(\{\psi\}) \geqslant \widehat{\eta}(\{0\})\,(1-\varepsilon').$$

This shows that $(\varLambda' - \varLambda')^{\varepsilon'} \subseteq \mathcal{I}_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-\varepsilon')\bigr)$.

Now, by Lemma 5.6.9, we have $(\varLambda')^{\varepsilon'} \subseteq (\varLambda' - \varLambda')^{2\varepsilon'}$, and therefore

$$(\varLambda')^{\varepsilon} \subseteq \mathcal{I}_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr).$$

Also, since $\varLambda' \subseteq \varLambda'' = \mathcal{I}_{\varLambda}(a)^{\varepsilon}$, we have

$$\mathcal{I}_{\varLambda}(a) \subseteq (\mathcal{I}_{\varLambda}(a)^{\varepsilon})^{\varepsilon} \subseteq (\varLambda')^{\varepsilon} \subseteq \mathcal{I}_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr).$$

This proves that every a-visible Bragg peak of $\varLambda$ is a $\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr)$-visible Bragg peak of $\varLambda'$. The claim then follows from the relative denseness of $\mathcal{I}_{\varLambda}(a)$.

We now prove (ii). We showed in (i) that

$$\mathcal{I}_{\varLambda}(a) \subseteq \mathcal{I}_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr).$$

Proposition 5.9.21 implies that, for all $0 < b < \widehat{\gamma}(\{0\})$, the sets $\mathcal{I}_{\varLambda}(b)$ are model sets in the same CPS. Therefore, for all $0 < b, c < \widehat{\gamma}(\{0\})$, there exists a finite set $F_{b,c}$ such that

$$\mathcal{I}_{\varLambda}(b) \subseteq \mathcal{I}_{\varLambda}(c) \mathbin{\hat{+}} F_{b,c} \quad \text{and} \quad \mathcal{I}_{\varLambda}(c) \subseteq \mathcal{I}_{\varLambda}(b) \mathbin{\hat{+}} F_{b,c}.$$

Since $\varLambda'$ is a regular model set, it is a pure point diffractive Meyer set. Hence, by Corollary 5.9.15, for all $0 < b < \widehat{\eta}(\{0\})$, the set $\mathcal{I}_{\varLambda'}(b)$ is relatively dense. It thus follows from Proposition 5.9.21 that, for all $0 < b < \widehat{\eta}(\{0\})$, the sets $\mathcal{I}_{\varLambda'}(b)$ are model sets in the same CPS. Hence, for all $0 < b, c < \widehat{\eta}(\{0\})$, there exists a finite set $F'_{b,c}$ such that

$$\mathcal{I}_{\varLambda'}(b) \subseteq \mathcal{I}_{\varLambda'}(c) \mathbin{\hat{+}} F'_{b,c} \quad \text{and} \quad \mathcal{I}_{\varLambda'}(c) \subseteq \mathcal{I}_{\varLambda'}(b) \mathbin{\hat{+}} F'_{b,c}.$$

Moreover, we also know that $\mathcal{I}_{\varLambda}(a) \subseteq \mathcal{I}_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr)$, that $\mathcal{I}_{\varLambda}(a)$ is relatively dense and that $\mathcal{I}_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr)$ has finite local complexity. Therefore, there exists a finite set F such that

$$\mathcal{I}_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr) \subseteq \mathcal{I}(a) \mathbin{\hat{+}} F.$$

Select any $0 < b < \widehat{\gamma}(\{0\})$ and $0 < c < \widehat{\eta}(\{0\})$. Setting $F_1 := F_{a,b}$ and $F_2 := F'_{c,\widehat{\eta}(\{0\})(1-2\varepsilon)}$, we obtain

$$\mathcal{I}_{\varLambda}(b) \subseteq \mathcal{I}_{\varLambda}(a) \mathbin{\hat{+}} F_1 \subseteq \mathcal{I}_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr) \mathbin{\hat{+}} F_1 \subseteq \mathcal{I}_{\varLambda'}(c) \mathbin{\hat{+}} F_1 \mathbin{\hat{+}} F_2$$

and

$$\mathcal{I}_{\varLambda'}(c) \subseteq I_{\varLambda'}\bigl(\widehat{\eta}(\{0\})(1-2\varepsilon)\bigr) \mathbin{\hat{+}} F_2 \subseteq \mathcal{I}_{\varLambda}(a) \mathbin{\hat{+}} F \mathbin{\hat{+}} F_2 \subseteq \mathcal{I}_{\varLambda}(b) \mathbin{\hat{+}} F_1 \mathbin{\hat{+}} F \mathbin{\hat{+}} F_2,$$

which completes the proof. □

5.10. More on Bragg spectra of Meyer sets

Here, we will use the properties of almost periodic measures to further study the Bragg spectrum of measures with Meyer set support. Below, for background details, we shall often use results from Chapter 4 in this volume [33], and we expect the reader to be familiar with this material.

We start by proving that, given a weighted Dirac comb ω with Meyer set support and autocorrelation γ, the strong almost periodic part γ_{s} of γ and its Bragg diffraction $\widehat{\gamma}_{\mathsf{pp}}$ are weighted model combs.

Proposition 5.10.1. *Let ω be any weighted Dirac comb on a σ-compact LCAG G. Assume that ω has Meyer set support and let γ be an autocorrelation of ω. Then, there exists a CPS $(G, H, \mathcal{L})$ and a function $g \in C_{\mathsf{c}}(H)$ so that $\gamma_{\mathsf{s}} = \omega_g$. Furthermore, there exists a CPS $(\widehat{G}, H_{\mathsf{fd}}, \mathcal{L}_{\mathsf{fd}})$ and a continuous function $g_{\mathsf{fd}} \in C_0(H_{\mathsf{fd}})$ which captures the pure point diffraction of ω via $\widehat{\gamma}_{\mathsf{pp}} = \omega_{g_{\mathsf{fd}}}$.*

Proof. By Theorem 5.8.1, there exists a model set $\varGamma$ such that

$$\operatorname{supp}(\gamma_{\mathsf{s}}) \subseteq \varGamma \quad \text{and} \quad \operatorname{supp}(\gamma_0) \subseteq \varGamma.$$

As γ_{s} is strongly almost periodic and $\varGamma$ is a Meyer set, Theorem 5.5.2 implies that there exists a CPS $(G, H, \mathcal{L})$ and a function $g \in C_{\mathsf{c}}(H)$ with $\gamma_{\mathsf{s}} = \omega_g$.

Furthermore, by Proposition 5.9.8, there exists a real number $C > 0$ such that, for all $\varepsilon > 0$,

$$\varDelta^{\varepsilon/C} \subseteq P_{\varepsilon}^{\infty}\bigl(\widehat{\gamma}_{\mathsf{pp}}\bigr).$$

Hence, the measure $\widehat{\gamma}_{\mathsf{pp}}$ is a sup-almost periodic pure point measure. The last claim now follows from Theorem 5.4.2. □

Later in this section, in Theorem 5.10.10, we will demonstrate that we can obtain the results from Proposition 5.10.1 with the two CPSs being dual to each other.

Remark 5.10.2.

(i) If $\varLambda$ is a Meyer set and $\omega = \delta_{\varLambda}$, then, in Proposition 5.10.1, we have $g \geqslant 0$ and both g and g_{fd} are non-trivial.
In general, this is not the case. For example, if ω is the ± 1 weighted Thue–Morse chain (compare [AO1, Sec. 4.6]), we have both $\gamma_{\mathsf{s}} = 0$ and $\widehat{\gamma}_{\mathsf{pp}} = 0$. In this case, we get $g \equiv 0$ and $g_{\mathsf{fd}} \equiv 0$.

(ii) Let $\varGamma$ be a regular model set, or a weak model set of maximal density [4, 18], with autocorrelation η. Let $(G, H, \mathcal{L})$ be the corresponding CPS and W the window for $\varGamma$. Let $(\widehat{G}, \widehat{H}, \mathcal{Z})$ be the dual CPS. Then, the covariogram of the window $g = 1_W * \widetilde{1_W}$ is in $C_{\mathsf{c}}(H)$, its Fourier transform $\widehat{g}$ is in $C_0(\widehat{H})$, and we have [5, 38, 4, 18]

$$\eta_{\mathsf{s}} = \eta = \omega_g \quad \text{and} \quad \widehat{\eta}_{\mathsf{pp}} = \widehat{\eta} = \omega_{\widehat{g}}.$$

In Proposition 5.10.1, we showed that similar results hold for the strongly almost periodic part of the autocorrelation and for the pure point part of the diffraction measure of a (weighted comb supported on a) Meyer set.

Next, we will see some consequences of Proposition 5.10.1.

Corollary 5.10.3. *Let $\varLambda$ be a Meyer set in a σ-compact LCAG and γ an autocorrelation of $\varLambda$.*

(i) *For all $0 < a < \widehat{\gamma}(\{0\})$, the sets $\mathcal{I}(a)$ of a-visible Bragg peaks are model sets in the same CPS.*

(ii) *The set* $\operatorname{supp}(\gamma_{\mathsf{s}})$ *is a model set.*

Proof. Let $(G, H, \mathcal{L}), g \in C_{\mathsf{c}}(H)$ and $(\widehat{G}, H_{\mathsf{fd}}, \mathcal{L}_{\mathsf{fd}}), g_{\mathsf{fd}} \in C_0(H_{\mathsf{fd}})$ be as in Proposition 5.10.1.

We first prove (i). For each $a > 0$, define

$$W_a := \big\{h \in H_{\mathsf{fd}} : g_{\mathsf{fd}} \geqslant a\big\}.$$

Since $a > 0$ and g_{fd} vanishes at infinity, the set W_a is compact. Moreover, as g_{fd} is continuous and $a < \widehat{\gamma}(\{0\}) = g_{\mathsf{fd}}(0)$, the set W_a has non-empty interior.

An easy computation shows that, in the CPS $(\widehat{G}, H_{\mathsf{fd}}, \mathcal{L}_{\mathsf{fd}})$, we have

$$\mathcal{I}(a) = \curlywedge(W_a),$$

which proves (i).

To prove (ii), let us observe that $W := \big\{h \in H : g(x) > 0\big\}$ is an open set with compact closure. Let as also note that γ is positive and hence so is γ_{s} by Proposition 4.10.11. This implies that $g \geqslant 0$, and hence, by Corollary 5.9.3, we have $W \neq \varnothing$.

Moreover, by Proposition 5.10.1, we have

$$\operatorname{supp}(\gamma_{\mathsf{s}}) = \curlywedge(W),$$

where $\curlywedge(W)$ is the model set defined by the window W in $(G, H, \mathcal{L})$. □

If $\varLambda$ is a repetitive Meyer set with pure point diffraction, we have that $\operatorname{supp}(\gamma) = \operatorname{supp}(\gamma_{\mathsf{s}}) = \varLambda - \varLambda$. This establishes the following result.

Corollary 5.10.4. *Let $\varLambda$ be a repetitive Meyer set in a σ-compact LCAG and assume that $\varLambda$ has pure point diffraction. Then, $\varLambda - \varLambda$ is a model set.* □

In the remainder of this section, we study the Fourier transform of Fourier transformable measures of the form ω_g with g admissible. An important ingredient will be Theorem 4.10.14, which relates the pure point part of the Fourier transform with the mean of the measure multiplied by characters.

We start by reviewing some results by Lenz and Richard [25].

Definition 5.10.5. Let $(G, H, \mathcal{L})$ be a CPS. A function $g : H \longrightarrow \mathbb{C}$ is called *admissible* if it is measurable, locally bounded and if, for all $\varepsilon > 0$ and $\phi \in C_{\mathsf{c}}(G)$, there exists a compact set $K \subseteq H$ so that, for all $(s,t) \in G \times H$, we have

$$\sum_{(t,h)\in\mathcal{L}} \bigl|\phi(t+s)\, g(h+k)\bigr| \bigl(1 - 1_K(h+k)\bigr) \leqslant \varepsilon.$$

It is obvious that any $g \in C_{\mathsf{c}}(H)$ is admissible.

Theorem 5.10.6 ([25, Thm. 3.1 and Thm. 3.3])**.** *Let $(G, H, \mathcal{L})$ be a CPS, with G being σ-compact, and let the function $g\colon H \longrightarrow \mathbb{C}$ be admissible. Let $(\widehat{G}, \widehat{H}, \mathcal{Z})$ be the corresponding dual CPS. Then, one has:*

(i) *The measure ω_g is strongly almost periodic.*

(ii) *If $(\chi, \chi^\star) \in \mathcal{Z}$, the limit*

$$c_\chi \,=\, \lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \sum_{(s,s^\star)\in\mathcal{L}} \chi(s)\, g(s^\star) \,=\, M(\chi\omega_g)$$

exists and satisfies

$$c_\chi \,=\, \operatorname{dens}(\mathcal{L}) \int_H \overline{\chi^\star}(h)\, g(h)\, \mathrm{d}\theta_H(h).$$

(iii) *Let γ be an autocorrelation of ω_g. Then, $\widehat{\gamma}$ is a pure point measure and satisfies*

$$\widehat{\gamma} \,=\, \sum_{(\chi,\chi^\star)\in\mathcal{Z}} \bigl|c_\chi\bigr|^2 \delta_\chi.$$ □

An immediate consequence of Theorem 5.10.8 is that a Meyer set has exactly the same set of Bragg peaks as a weighted model set, in the following sense.

Corollary 5.10.7. *Let $\varLambda$ be a Meyer set in a σ-compact LCAG G and let γ be an autocorrelation of $\varLambda$. Then, there exists a CPS $(G, H, \mathcal{L})$, a regular model set $\varGamma := \curlywedge(W)$ and a function $g \in C_{\mathsf{c}}(H)$ such that, for the weighted*

Dirac comb ω on the model set $\varGamma$ defined by

$$\omega := \sum_{x\in\varGamma} g(x^\star)\,\delta_x$$

with autocorrelation η, we have

$$\widehat{\eta}(\{\chi\}) = \bigl[\widehat{\gamma}(\{\chi\})\bigr]^2.$$

In particular, ω and $\varLambda$ have the same set of Bragg peak positions.

Proof. We know that γ_{s} is a continuous weighted model comb supported on a Meyer set. Thus, by Theorem 5.5.2, there exists a CPS $(G, H, \mathcal{L})$ and a function $g \in C_{\mathsf{c}}(H)$ so that $\gamma_{\mathsf{s}} = \omega_g$.

Let W be any compact set in H such that $\operatorname{supp}(g) \subseteq W^\circ$, and define $\varGamma := \curlywedge(W)$. Then,

$$\omega_g = \gamma_{\mathsf{s}} = \sum_{x\in\varGamma} g(x^\star)\,\delta_x.$$

As $g \in C_{\mathsf{c}}(H)$, it follows that g is admissible. Thus, by Theorem 5.10.8(iii) and Theorem 4.10.14 (compare also [28, Thm. 7.6]), we have

$$\widehat{\eta}(\{\chi\}) = \bigl[\widehat{\omega_g}(\{\chi\})\bigr]^2 = \bigl[\widehat{\gamma}(\{\chi\})\bigr]^2,$$

which completes the proof. □

Another consequence of Theorem 5.10.8 is the following result.

Proposition 5.10.8. *Let $(G, H, \mathcal{L})$ be a CPS with G being σ-compact, and let $g \in L^1(H)$ be admissible. Let $(\widehat{G}, \widehat{H}, \mathcal{Z})$ be the dual CPS. If ω_g is Fourier transformable, then the following statements hold,*

(i) $\widehat{\omega_g} = \operatorname{dens}(\mathcal{L})\,\omega_{\breve{g}}$;

(ii) $\widehat{\omega_g}$ *is sup-almost periodic;*

(iii) ω_g *is positive definite if and only if g is positive definite.*

Proof. We start by proving (i). By Theorem 5.10.6, ω_g is strongly almost periodic, thus $\widehat{\omega_g}$ is pure point by Corollary 4.10.13.

Hence, by Theorem 4.10.14, we have

$$\widehat{\omega_g}(\{\chi\}) = M(\overline{\chi}\,\omega_g)$$

for all $\chi \in \widehat{G}$. Therefore, for all $(\chi, \chi^\star) \in \mathcal{Z}$, we obtain

$$\widehat{\omega_g}(\{\chi\}) = \operatorname{dens}(\mathcal{L}) \int_H g(h)\,\overline{\chi^\star(h)}\,\mathrm{d}\theta_H(h) = \operatorname{dens}(\mathcal{L})\,\breve{g}(\chi^\star).$$

To complete the proof of (i), we need to show that, for all $\chi \notin \pi_1(\mathcal{Z})$, we have $\widehat{\omega_g}(\chi) = 0$.

Let γ be the autocorrelation of ω_g. Since ω_g is strongly almost periodic, the limit

$$c_\chi \;=\; \lim_{n\to\infty} \frac{1}{\theta_G(B_n)} \sum_{s\in L\cap B_n} \chi(s)\, \omega_g(s)$$

exists for every van Hove sequence $\{B_n\}$ and for all $\chi \in \widehat{G}$. Then, by Theorem 5.10.6(iii) (see also [25, 14]), we have

$$\widehat{\gamma}(\{\chi\}) \;=\; |c_\chi|^2 \;=\; |\widehat{\omega_g}(\chi)|^2.$$

Now, again by Theorem 5.10.6(iii), we have $\widehat{\gamma}(\chi) = 0$ for all $\chi \notin \pi_1(\mathcal{Z})$, and thus $|\widehat{\omega_g}(\chi)|^2 = 0$.

To prove (ii), note that $\operatorname{dens}(\mathcal{L})\, \omega_{\breve{g}}$ is the Fourier transform of $\widehat{\omega_g}$, and thus translation bounded by Theorem 4.9.23. Moreover, $\breve{g} \in C_0(\widehat{H})$, so $\widehat{\omega_g}$ is sup-almost periodic by Theorem 5.4.2.

Finally, we show (iii). We have that ω_g is positive definite if and only if $\widehat{\omega_g} = \operatorname{dens}(\mathcal{L})\, \omega_{\breve{g}}$ is positive. Also, g is positive definite if and only if $\breve{g}$ is positive. Since $\breve{g}$ is continuous and $\pi_2(\mathcal{Z})$ is dense in H, we get that $\breve{g}$ is positive if and only if $\omega_{\breve{g}}$ is positive, which completes the proof. □

Remark 5.10.9. Let us note that, as noted in [4], part (iii) of Proposition 5.10.8 does not really require the Fourier transformability of ω_g. Indeed, if ω_g is positive definite as a measure, it is automatically Fourier transformable, and the direct implication works. Furthermore, if g is positive definite as a function, it is straightforward to check that the function $f\colon L \longrightarrow \mathbb{C}$ defined by $x \mapsto f(x) := g(x^\star)$ is positive definite as well. Consequently, by [27, Prop. 2.4], the measure ω_g is positive definite on $L \subseteq G$, and hence on G_{d} by [27, Lemma 2.10]. Then, the claim follows from [27, Prop. 2.4]. ♢

We are now able to prove that the results in Proposition 5.10.1 can be obtained for a dual pair of CPSs.

Theorem 5.10.10. *Let $\varLambda \subseteq G$ be a Meyer set, with G a σ-compact LCAG, and let γ be an autocorrelation of $\varLambda$. Then, there exists a CPS $(G, H, \mathcal{L})$ and a function $g \in C_{\mathsf{c}}(H)$ so that*

$$\gamma_{\mathsf{s}} \;=\; \omega_g \quad \textit{and} \quad \widehat{\gamma}_{\mathsf{pp}} \;=\; \operatorname{dens}(\mathcal{L})\, \omega_{\breve{g}}.$$

Proof. The existence of the CPS and of the function g with $\gamma_{\mathsf{s}} = \omega_g$ follows from Proposition 5.10.1.

Since $g \in C_{\mathsf{c}}(H)$, one has $g \in L^1(H)$ with g admissible. Thus, by Proposition 5.10.8, we have $\widehat{\gamma}_{\mathsf{pp}} = \operatorname{dens}(\mathcal{L})\, \omega_{\breve{g}}$ in the dual CPS. □

We complete the section by introducing a recent result which complements Proposition 5.10.8.

Theorem 5.10.11 ([38, Thm. 5.3]). *Consider a CPS $(G, H, \mathcal{L})$ with G being a σ-compact LCAG, and let $g \in C_{\mathsf{c}}(H)$. Let $(\widehat{G}, \widehat{H}, \mathcal{Z})$ be the corresponding dual CPS. Then, the measure ω_g is Fourier transformable if and only if one has $\check{g} \in L^1(\widehat{H})$. Moreover, we have $\widehat{\omega_g} = \operatorname{dens}(\mathcal{L})\, \omega_{\check{g}}$ in this case.* □

Note that Theorem 5.10.11 characterises the Fourier transformability of ω_g for $g \in C_{\mathsf{c}}(G)$. In general, however, it is unclear which admissible functions g on H define Fourier transformable measures ω_g. A necessary condition is $\check{g} \in L^1(\widehat{H})$ [38, Lemma 5.2], but it is not clear whether this is also sufficient.

5.11. Concluding remarks

The Baake–Moody construction of a CPS is becoming a powerful tool in the study of model sets and Meyer sets, with applications in many seemingly unrelated areas. Introduced in [7], it was a key ingredient in the classification of regular model sets via dynamical systems [6]. Also, in our current work, it was the key to both the classification of norm- and sup-almost periodic measures in terms of CPSs, and the classification of Meyer sets in terms of ε-dual characters. The appearance of this construction in so many different situations is surprising, and one can only wonder what other applications it might have in the future, and if there might be a deeper reason why this construction can be used in so many different situations.

The classifications of norm- and sup-almost periodic, weighted Dirac combs turned out to be unexpectedly simple. However, it also led to some interesting new questions. For example, given a CPS $(G, H, \mathcal{L})$, it would be very helpful to find all functions $g \in C_0(H)$ which define translation bounded measures ω_g on G.

Also, given an arbitrary norm-almost periodic measure μ with locally finite sets of almost periods, we can apply the Baake–Moody construction to the sets $P_\varepsilon^K(\mu)$. In the corresponding CPS, the sets $P_\varepsilon^K(\mu)$ are model sets, but it is currently unclear whether one can recover the measure μ from the CPS.

While strong almost periodicity is very important for long-range order because of its connection with pure point diffraction, this work suggests that norm- and sup-almost periodicity might be more suitable concepts for sets and measures produced by CPSs. Therefore, norm-almost periodicity becomes a very interesting and useful concept: It is stronger than strong almost periodicity, hence implies pure point diffractivity, and it also leads to the construction of a CPS. Moreover, for measures supported inside Meyer sets, strong and norm-almost periodicity are equivalent.

A famous question of Lagarias [23] asked whether, given a point set $\varLambda$ which is repetitive, has FLC and pure point diffraction, it follows that $\varLambda$ is a

Meyer set. This question was recently answered in the negative by Kellendonk and Sadun [17]. Our above discussion suggests that, in order to obtain the Meyer condition, norm-almost periodicity of the autocorrelation is a more natural assumption than pure point diffraction. This leads to the following question: Given a point set $\varLambda$ which is repetitive, has finite local complexity and an autocorrelation which is norm-almost periodic — does it follow that $\varLambda$ is a Meyer set?

Using the Baake–Moody construction and properties of almost periodic measures, we were able to extend the classification of Meyer sets from $\mathbb{R}^d$ to an arbitrary LCAG, except for the Lagarias condition that $\varLambda - \varLambda$ is uniformly discrete. Instead, we had to use the seemingly stronger condition that the set $\varLambda - \varLambda - \varLambda$ is locally finite. It is currently unclear whether this stronger condition is really needed for non-compactly generated LCAGs, or whether the methods used above are not strong enough to prove this equivalence in general.

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5.A. Appendix. Harmonious sets

In this appendix, we review Meyer's proof [29] of Theorem 5.A.2 (see below) in the context of metrisable LCAGs. Meyer's original proof was in the context of separable metrisable groups, but we will see that his proof does not require separability. Our proof closely follows that of [30].

For the entire section, we will denote the dual group of G_{d} by $\widehat{G}_{\mathrm{B}}$. As we have seen in Section 4.2, this group is the *Bohr compactification* of $\widehat{G}$ and is a compact group. We should note here that Meyer [29] and Moody [30] use the notation $(\widehat{G})_{\mathrm{alg}}$ for the Bohr compactification of G, as it represents the group of algebraic characters on G. We prefer the notation $\widehat{G}_{\mathrm{B}}$, as it is the standard notation in this book.

We start by recalling the concept of harmonious set.

Definition 5.A.1. Let G be an LCAG, let $\varLambda \subseteq G$ and let $\varepsilon > 0$. We say that $\varLambda$ is *ε-harmonious*, if, for every algebraic character $\psi \in \widehat{G}_{\mathrm{B}}$, there exists

a continuous character $\chi \in \widehat{G}$ such that, for all $x \in \Lambda$, we have

$$|\psi(x) - \chi(x)| < \varepsilon.$$

We say that Λ is *harmonious* if Λ is ε-harmonious for all $\varepsilon > 0$.

We can now prove that, in any metrisable LCAG, a set Λ is ε-harmonious precisely when the set Λ^ε of ε-dual characters is relatively dense.

Theorem 5.A.2. *Let G be a metrisable LCAG, let $\Lambda \subseteq G$ and $\varepsilon > 0$. Then, Λ^ε is relatively dense if and only if Λ is ε-harmonious.*

Proof. For each $\varepsilon > 0$, we define

$$V^\varepsilon(\Lambda) := \big\{\chi \in \widehat{G}_{\mathrm{B}} : |\chi(x) - 1| \leqslant \varepsilon \text{ for all } x \in \Lambda\big\}.$$

Then, Λ is ε-harmonious if and only if

$$V^\varepsilon(\Lambda) \mathbin{\hat{+}} \widehat{G} = \widehat{G}_{\mathrm{B}}.$$

We first prove the implication $\Longrightarrow$. Since G is an LCAG, so is $\widehat{G}$. Let $K \subseteq \widehat{G}$ be a compact set such that $\Lambda^\varepsilon \mathbin{\hat{+}} K = \widehat{G}$. Using $\Lambda^\varepsilon = V^\varepsilon(\Lambda) \cap \widehat{G}$, we get that

$$\widehat{G} \subseteq V^\varepsilon(\Lambda) \mathbin{\hat{+}} K \subseteq \widehat{G}_{\mathrm{B}}.$$

Since K is compact in $\widehat{G}$ and since the embedding $\widehat{G} \hookrightarrow \widehat{G}_{\mathrm{B}}$ is continuous, K is also compact in $\widehat{G}_{\mathrm{B}}$. By definition, $V^\varepsilon(\Lambda)$ is closed and hence compact in $\widehat{G}_{\mathrm{B}}$. Therefore, $V^\varepsilon(\Lambda) \mathbin{\hat{+}} K$ is compact and hence closed in $\widehat{G}_{\mathrm{B}}$. Consequently, $V^\varepsilon(\Lambda) \mathbin{\hat{+}} K$ is closed in $\widehat{G}_{\mathrm{B}}$ and contains the dense subset $\widehat{G}$. This implies that

$$V^\varepsilon(\Lambda) \mathbin{\hat{+}} K = \widehat{G}_{\mathrm{B}},$$

which shows our implication.

We now prove the other implication. As G is a metrisable LCAG, $\widehat{G}$ is a σ-compact group [36, Thm. 4.2.7]. Therefore, we can find a sequence $\{K_n\}$ of compact sets such that $0 \in K_1$, $K_n \subseteq K_{n+1}^\circ$ and $\widehat{G} = \bigcup_n K_n$. Then,

$$\widehat{G}_{\mathrm{B}} = V^\varepsilon(\Lambda) \mathbin{\hat{+}} \widehat{G} = \bigcup_n \big(V^\varepsilon(\Lambda) \mathbin{\hat{+}} K_n\big).$$

Again, the continuity of $\widehat{G} \hookrightarrow \widehat{G}_{\mathrm{B}}$ implies that K_n is also compact in $\widehat{G}_{\mathrm{B}}$. Then, $V^\varepsilon(\Lambda) \mathbin{\hat{+}} K_n$ is compact and hence closed in $\widehat{G}_{\mathrm{B}}$.

Since $\widehat{G}_{\mathrm{B}}$ is a locally compact Hausdorff space, the Baire category theorem [10] implies the existence of an n such that $V^\varepsilon(\Lambda) \mathbin{\hat{+}} K_n$ has non-empty interior. Therefore, as the embedding $\widehat{G} \hookrightarrow \widehat{G}_{\mathrm{B}}$ has dense image,

$$\widehat{G} \mathbin{\hat{+}} \big(V^\varepsilon(\Lambda) \mathbin{\hat{+}} K_n\big) = \widehat{G}_{\mathrm{B}}.$$

As the left-hand side is an open cover of the compact set $\widehat{G}_{\mathrm{B}}$ by translates of the set open set $(V^{\varepsilon}(\varLambda) \mathbin{\hat{+}} K_n)^{\circ}$, there exists a finite set $F \subseteq \widehat{G}$ such that

$$F \mathbin{\hat{+}} \bigl(V^{\varepsilon}(\varLambda) \mathbin{\hat{+}} K_n\bigr) \,=\, \widehat{G}_{\mathrm{B}}.$$

Let $K = F \mathbin{\hat{+}} K_n$. Then, K is compact in $\widehat{G}$, and we will show that

$$\varLambda^{\varepsilon} \mathbin{\hat{+}} K \,=\, \widehat{G}.$$

Indeed, let $\chi \in \widehat{G}$. Then, we can write $\chi = \psi \mathbin{\hat{+}} \phi \mathbin{\hat{+}} \nu$ with $\psi \in F$, $\phi \in V^{\varepsilon}(\varLambda)$ and $\nu \in K_n$. By the definition of K, we have $\psi \mathbin{\hat{+}} \nu \in K$. Moreover, we have $\phi = \chi \mathbin{\hat{-}} \psi \mathbin{\hat{-}} \nu$ and thus $\phi \in \widehat{G}$. This shows that

$$\chi \,=\, \phi \mathbin{\hat{+}} (\psi \mathbin{\hat{+}} \nu), \quad \phi \,\in\, \widehat{G} \cap V^{\varepsilon}(\varLambda) \,=\, \varLambda^{\varepsilon}, \quad \psi \mathbin{\hat{+}} \nu \,\in\, K,$$

which completes the proof. □

Corollary 5.A.3. *Let $\varLambda$ be relatively dense in a metrisable LCAG G. Then, $\varLambda$ is harmonious if and only if $\varLambda^{\varepsilon}$ is relatively dense for all $\varepsilon > 0$.* □

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CHAPTER 6

Averaging Almost Periodic Functions along Exponential Sequences

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This short chapter may be viewed as a complement to the chapters on almost periodicity. Its goal is a fairly self-contained account of some averaging processes of functions along sequences of the form $(\alpha^n x)_{n\in\mathbb{N}}$, where α is a fixed real number with $|\alpha| > 1$ and $x \in \mathbb{R}$ is arbitrary. Such sequences appear in the spectral theory of inflation systems in various ways. Due to the connection with uniform distribution theory, the results will mostly be *metric* in nature, which means that they hold for Lebesgue-almost every $x \in \mathbb{R}$.

6.1. Introduction

A frequently encountered problem in mathematics and its applications is the study of averages of the form $\frac{1}{N}\sum_{n=1}^{N} f(x_n)$, where f is a function with values in $\mathbb{C}$ or, more generally, in some Banach space, and $(x_n)_{n\in\mathbb{N}}$ is a sequence of numbers in the domain of f. Quite often, an exact treatment of these averages is out of hand, and one resorts to the analysis of asymptotic properties for large N. This, for instance, is common in analytic number theory; compare [18, 19, 1] and references therein. Equally important is the case where one can establish the existence of a limit as $N \to \infty$, and then calculate it. This occupies a good deal of ergodic theory, where Birkhoff's theorem and Kingman's subadditive theorem provide powerful tools to tackle the problem; see [14, 37] for background.

However, not all tractable cases present themselves in a way that is immediately accessible to tools from ergodic theory. Also, depending on the nature of the underlying problem, one might prefer a more elementary method, as Birkhoff-type theorems already represent a fairly advanced kind of 'weaponry'. An interesting (and certainly not completely independent) approach is provided by the theory of uniform distribution of sequences, which essentially goes back to Weyl [38] and has emerged as a major tool for the

study of function averages, in particular for functions that are periodic or defined on a compact domain; see [24, 16, 25] and references therein for more.

In this contribution, we recall some of these concepts, with an eye on both methods (uniform distribution and ergodic theory), and use the tools to treat averages of almost periodic functions along sequences where this makes sense, in particular along sequences of the form $(\alpha^n x)_{n\in\mathbb{N}}$ with 'generic' $x \in \mathbb{R}$ and a fixed number $\alpha \in \mathbb{R}$ with $|\alpha| > 1$. The first subtlety that we shall encounter here emerges when α is not an integer, which requires some care for functions that fail to be locally Riemann-integrable. The second subtlety occurs when we extend our considerations to almost periodic functions.

While the latter extension represents a relatively simple step beyond periodic functions as long as one retains almost periodicity in the sense of Bohr, matters become more involved when singularities occur or weaker notions of almost periodicity are needed. Below, we shall discuss some extensions of this kind that are relevant in practice; compare [17] for some related results. Let us note that some of the notions and concepts used below are studied in much greater generality in Chapters 4 and 5 of this volume [28, 35].

Before we begin our exposition, let us mention that averages of 1-periodic functions are often just the first step in the study of Riesz–Raikov sums, that is, sums of the form $\sum_{k=0}^{n-1} f(\alpha^k t)$. Kac's investigation for $\alpha = 2$ in [21] and Takahashi's refined and generalised analysis [36] are early examples that consider limits (in a law of large numbers scaling) as well as distributions (in a central limit theorem scaling, when $\int_0^1 f(t)\,\mathrm{d}t = 0$). This led to a more elaborate derivation of central limit theorems for Riesz–Raikov sums along exponential sequences; compare [30, 26, 32] and references therein.

Below, we are mainly interested in the Birkhoff-type averages, with a focus on functions that fail to be periodic, but still have some repetitivity structure in the form of a suitable almost periodicity. In this sense, we have selected one particular aspect of Riesz–Raikov sums that appears in the theory of aperiodic order [AO1, 9, 2].

6.2. Preliminaries and general setting

As far as possible, we follow the general (and fairly standard) notation from [AO1, Ch. 1], wherefore only deviations or extensions will be mentioned explicitly. In particular, we will use the Landau symbols $\mathcal{O}$ and o for the standard asymptotic behaviour of real- or complex-valued functions; compare [1, 18] for definitions and examples.

When two sets $A, B \subseteq \mathbb{R}$ are given, we denote their *Minkowski sum* as $A + B := \{a + b : a \in A,\, b \in B\}$. In particular, if the point set $S \subset \mathbb{R}$ is locally finite and $\varepsilon > 0$, we use $S + (-\varepsilon, \varepsilon)$ for the open subset of $\mathbb{R}$ that

emerges from S as $\bigcup_{x\in S}(x-\varepsilon, x+\varepsilon)$. Note that its complement in $\mathbb{R}$ is then a closed set (possibly empty).

Below, we frequently talk about results of metric nature, where Lebesgue measure λ on $\mathbb{R}$ is our reference measure. When a statement is true for almost every $x \in \mathbb{R}$ with respect to Lebesgue measure, we will simply say that it holds for a.e. $x \in \mathbb{R}$. Likewise, when we speak of a null set, we mean a null set with respect to Lebesgue measure.

Recall that a sequence $(x_n)_{n\in\mathbb{N}}$ of real numbers is called *uniformly distributed modulo* 1 if, for all real numbers a, b with $0 \leqslant a < b \leqslant 1$, we have

$$\lim_{N\to\infty} \frac{1}{N} \operatorname{card}\Bigl([a,b) \cap \bigl\{\langle x_1\rangle, \ldots, \langle x_N\rangle\bigr\}\Bigr) \,=\, b-a,$$

where $\langle x\rangle$ denotes the fractional part[1] of $x \in \mathbb{R}$. We refer to [24, 10] for general background. Recall that a function f on $\mathbb{R}$ is 1-*periodic* if $f(x+1) = f(x)$ holds for all $x \in \mathbb{R}$. One fundamental result, due to Weyl [38], can now be formulated as follows; see also [19, Thm. 5.3].

Lemma 6.2.1 (Weyl's criterion)**.** *For a sequence $(x_n)_{n\in\mathbb{N}}$ of real numbers, the following properties are equivalent.*

(1) *The sequence is uniformly distributed modulo* 1*.*

(2) *For every complex-valued,* 1*-periodic continuous function f, one has*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(x_n) \,=\, \int_0^1 f(x)\,\mathrm{d}x.$$

(3) *The relation from* (2) *holds for every* 1*-periodic function that is locally Riemann-integrable.*

(4) *The relation*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \mathrm{e}^{2\pi \mathrm{i} k x_n} \,=\, \delta_{k,0}$$

holds for every $k \in \mathbb{Z}$. □

Let us note in passing that the equivalence of conditions (1) and (2) can also be understood in terms of systems of almost invariant integrals and Eberlein's ergodic theorem. These notions are reviewed and studied in some detail in Chapter 4 of this volume.

Remark 6.2.2. Weyl's criterion (which is also known as Weyl's lemma) is an important tool for calculating the average of a locally Riemann-integrable periodic function along a uniformly distributed sequence. In fact, a 1-periodic function is locally Riemann-integrable if and only if the Birkhoff average

[1] Since we use $\{x\}$ for singleton sets, we resort to the less common notation $\langle x\rangle$ for the fractional part of x in order to avoid misunderstandings.

converges for *every* sequence that is uniformly distributed modulo 1; compare [15] as well as [19, p. 123].

Conversely, the integral of a Riemann-integrable function can be approximated by averages along uniformly distributed sequences. This is a standard method in numerical integration, in particular for higher-dimensional integrals; see [20, 25] and references therein for more. ♢

There is an abundance of known results on uniformly distributed sequences and their finer properties; we refer to [24] for the classic theory and to [10] and references therein for more recent developments. Here, we are particularly interested in one specific class of sequences, for which the uniform distribution is well known; see [10, Thms. 1.7 and 1.10] as well as [14, Sec. 7.3, Thm. 1] or [24, Cor. 1.4.3 and Exc. 1.4.3].

Fact 6.2.3. *Consider the sequence* $(\alpha^n x)_{n\in\mathbb{N}}$. *For fixed* $\alpha \in \mathbb{R}$ *with* $|\alpha| > 1$, *it is uniformly distributed modulo* 1 *for a.e.* $x \in \mathbb{R}$. *For fixed* $0 \neq x \in \mathbb{R}$, *it is uniformly distributed modulo* 1 *for a.e.* $\alpha \in \mathbb{R}$ *with* $|\alpha| > 1$. □

Below, we will mainly be concerned with the first case, where a fixed α with $\alpha > 1$ or $|\alpha| > 1$ is given. This situation is of interest in the theory of aperiodic order, for instance in connection with the renormalisation analysis of inflation tiling systems, because it plays an important role for the averaging of functions with certain repetition properties along the real line.

Let us mention in passing that, when $\alpha = q \geqslant 2$ is an integer, $(q^n x)_{n\in\mathbb{N}}$ is uniformly distributed modulo 1 if and only if x is a *normal* number [10] in base q, which means that the q-ary expansion of x contains all possible finite substrings in the digit set $\{0, 1, \ldots, q-1\}$ in such a way that any substring of length ℓ has frequency $1/q^\ell$. In the Lebesgue sense, a.e. $x \in \mathbb{R}$ is normal with respect to all integer bases [10, Thm. 4.8], but it is a hard problem to decide on normality for any given number.

Remark 6.2.4. Consider a sequence $(u_n)_{n\in\mathbb{N}_0}$ of real numbers such that $\inf_{n\neq m} |u_n - u_m| > 0$. Then, by [24, Cor. 1.4.3], the sequence $(u_n x)_{n\in\mathbb{N}_0}$ is uniformly distributed modulo 1 for a.e. $x \in \mathbb{R}$. In fact, it is a rather direct consequence that, for any $k \in \mathbb{N}$, $\ell \in \mathbb{N}_0$ and any real number $L > 0$, the arithmetic progression sequence $(u_{km+\ell}\, x)_{m\in\mathbb{N}}$ is uniformly distributed modulo L for a.e. $x \in \mathbb{R}$. This is the *total Bohr ergodicity* of $(u_n)_{n\in\mathbb{N}_0}$ as introduced in [17, Def. 2.1]. Clearly, $u_n = \alpha^n$ with $|\alpha| > 1$ defines such a sequence, while no bounded sequence can have this property. ♢

As soon as we leave the realm of periodic functions that are locally Riemann-integrable, the desired averaging statements will need some finer properties of our sequences $(\alpha^n x)_{n\in\mathbb{N}}$, where we assume $|\alpha| > 1$ as before. In particular, we will need details on the uniform distribution (or the deviation

from it) and some information on the approximation or non-approximation of numbers in a given set by the sequence elements. For the first issue, we need the discrepancy structure of the sequence, and some Diophantine approximation properties for the latter.

Recall that the *discrepancy* of a sequence $(x_n)_{n\in\mathbb{N}}$ is quantified in terms of the first N elements of the sequence (taken modulo 1), namely by the number

$$\mathcal{D}_N \,:=\, \sup_{0\leqslant a<b\leqslant 1} \Big| \frac{1}{N} \operatorname{card}\Big([a,b) \cap \big\{ \langle x_1\rangle, \ldots, \langle x_N\rangle \big\} \Big) - (b-a) \Big| \,,$$

together with its asymptotic properties as $N \to \infty$.

In this terminology, the sequence $(x_n)_{n\in\mathbb{N}}$ is uniformly distributed modulo 1 if and only if $\lim_{N\to\infty} \mathcal{D}_N = 0$; see [10, Thm. 1.12]. The discrepancy of sequences is a huge research area in itself; see [16] and references therein for a comprehensive exposition. We will need the following result, where we refer to [19, Thm. 5.13] and [22] for proofs.

Fact 6.2.5. *Let $\alpha \in \mathbb{R}$ with $|\alpha| > 1$ be given. Then, for any fixed $\varepsilon > 0$, the discrepancy of the sequence $(\alpha^n x)_{n\in\mathbb{N}}$, for a.e. $x \in \mathbb{R}$, asymptotically is*

$$\mathcal{D}_N \,=\, \mathcal{O}\left(\frac{\big(\log(N)\big)^{\frac{3}{2}+\varepsilon}}{\sqrt{N}} \right)$$

as $N \to \infty$. □

Next, we need a *Diophantine approximation* property. If $\varnothing \neq Y \subset \mathbb{R}$ is a uniformly discrete point set, compare [AO1, Sec. 2.1], we can define

$$\operatorname{dist}(x, Y) \,:=\, \min_{y\in Y} |x-y|$$

as the distance of $x \in \mathbb{R}$ from Y. Now, one can state the following metric 'non-approximation' result, which is a versatile generalisation of the classic situation with $Y = \mathbb{Z}$.

Lemma 6.2.6. *Let $\alpha \in \mathbb{R}$ with $|\alpha| > 1$ be given, and let $Y \subset \mathbb{R}$ be a non-empty, uniformly discrete point set. Further, fix some $\varepsilon > 0$. Then, for a.e. $x \in \mathbb{R}$, the inequality*

$$\operatorname{dist}(\alpha^{n-1}x, Y) \,\geqslant\, \frac{1}{n^{1+\varepsilon}}$$

holds for almost all $n \in \mathbb{N}$, by which we mean that it holds for all natural numbers except at most finitely many.

Proof. The statement is trivial when Y is a finite point set, so let us assume that Y is unbounded. In this case, one still has

$$\delta \,:=\, \inf\big\{ |x-y| : x, y \in Y,\, x \neq y \big\} \,>\, 0,$$

due to the assumed uniform discreteness of Y. Consequently, the number of points of Y in an arbitrary interval $[a, b]$ with $a \leqslant b$ satisfies

$$\mathrm{card}\big(Y \cap [a,b]\big) \leqslant 1 + \Big[\frac{b-a}{\delta}\Big], \tag{6.2.1}$$

where $[.]$ is the Gauß bracket.

Let $m \in \mathbb{Z}$ be arbitrary, but fixed, and consider $I_m = [m, m+1]$. With $\mathbb{R} = \bigcup_{m\in\mathbb{Z}} I_m$, it suffices to show that our claim fails at most for a null set within the interval I_m, as the countable union of null sets is still a null set.

Choose $\varepsilon > 0$ and, for $n \in \mathbb{N}$, consider the set

$$A_n^{(m)} := \Big\{x \in I_m : \mathrm{dist}(\alpha^{n-1}x, Y) < \frac{1}{n^{1+\varepsilon}}\Big\}.$$

It is clearly measurable, and its measure, since $|\alpha| > 1$, can be estimated as

$$\begin{aligned}\lambda\big(A_n^{(m)}\big) &= \frac{1}{|\alpha|^{n-1}}\,\lambda\Big\{z \in \alpha^{n-1}I_m : \mathrm{dist}(z,Y) < \frac{1}{n^{1+\varepsilon}}\Big\}\\ &\leqslant \frac{1}{|\alpha|^{n-1}}\,\frac{2}{n^{1+\varepsilon}}\left(1 + \Big[\frac{|\alpha|^{n-1}}{\delta}\Big]\right) = \mathcal{O}\Big(\frac{1}{n^{1+\varepsilon}}\Big),\end{aligned}$$

where the second step is a consequence of Eq. (6.2.1). We thus know that there is a $C > 0$ such that $\lambda\big(A_n^{(m)}\big) \leqslant C/n^{1+\varepsilon}$ for all $n \in \mathbb{N}$.

Now, we have

$$0 \leqslant \sum_{n\geqslant 1} \lambda\big(A_n^{(m)}\big) \leqslant C \sum_{n\geqslant 1} \frac{1}{n^{1+\varepsilon}},$$

where the second sum is convergent, and thus also the first. Then, Cantelli's lemma[2] tells us that

$$E_\infty^{(m)} := \big\{x \in I_m : x \in A_n^{(m)} \text{ for infinitely many } n \in \mathbb{N}\big\}$$

is indeed a null set, which is what we needed to show. □

Remark 6.2.7. Though immaterial for the proof, it is often useful in an application to also remove all $x \in \mathbb{R}$ with $Y \cap \{\alpha^{n-1}x : n \in \mathbb{N}\} \neq \varnothing$, which constitutes a null set because it is clearly countable or even finite. ♢

The lower bound in Lemma 6.2.6 can be replaced by the values of a more general, non-negative arithmetic function, $\psi(n)$ say, provided one has the summability condition $\sum_{n\in\mathbb{N}} \psi(n) < \infty$. When this sum diverges, the situation changes. Indeed, for instance if $\alpha = 2$ and $Y = \mathbb{Z}$, there is then a set $X \subset \mathbb{R}$ of full measure such that, for $x \in X$, the distance of $2^{n-1}x$ from the nearest integer is smaller than $\frac{1}{n}$ for infinitely many $n \in \mathbb{N}$; see [3] for a more general result in this direction. Moreover, one cannot do better than

[2]This being the 'easy half' of the Borel–Cantelli lemma, which goes back to Cantelli, we follow [10, App. C] in our terminology, and also refer to this reference for a proof.

using some $\varepsilon > 0$ in Lemma 6.2.6, in line with the divergence of the harmonic series.

6.3. Averaging periodic functions

Let us first state a result that emerges from an application of Weyl's criterion to the special type of sequences we are interested in.

Fact 6.3.1. *Let $f\colon \mathbb{R} \longrightarrow \mathbb{C}$ be a continuous or, more generally, a locally Riemann-integrable function that is L-periodic, so $f(x+L) = f(x)$ holds for some fixed $L > 0$ and all $x \in \mathbb{R}$. If α is a real number with $|\alpha| > 1$, one has*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} f(\alpha^n x) \,=\, \frac{1}{L} \int_0^L f(y)\,\mathrm{d}y$$

for a.e. $x \in \mathbb{R}$.

Proof. Since any L-periodic continuous function is also locally Riemann-integrable, it suffices to consider the latter class. Define a new function g by $g(x) := f(Lx)$, which clearly is 1-periodic and locally Riemann-integrable. Now, we have

$$\frac{1}{N} \sum_{n=0}^{N-1} f(\alpha^n x) \,=\, \frac{1}{N} \sum_{n=0}^{N-1} g\bigl(\alpha^n \tfrac{x}{L}\bigr),$$

where $\bigl(\alpha^n \frac{x}{L}\bigr)_{n\in\mathbb{N}}$ is uniformly distributed modulo 1 for a.e. $\frac{x}{L} \in \mathbb{R}$, and hence also for a.e. $x \in \mathbb{R}$, by Fact 6.2.3. Consequently, Weyl's criterion from Lemma 6.2.1 tells us that

$$\frac{1}{N} \sum_{n=0}^{N-1} f(\alpha^n x) \;\xrightarrow{N\to\infty}\; \int_0^1 g(z)\,\mathrm{d}z \,=\, \frac{1}{L} \int_0^L f(y)\,\mathrm{d}y$$

holds for all such cases, which means for a.e. $x \in \mathbb{R}$ as claimed. □

Note that one can rewrite Fact 6.3.1 with the *mean* of f, because

$$M(f) \,:=\, \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} f(y)\,\mathrm{d}y \,=\, \lim_{T\to\infty} \frac{1}{T} \int_a^{a+T} f(y)\,\mathrm{d}y \,=\, \frac{1}{L} \int_0^L f(y)\,\mathrm{d}y$$

holds for every L-periodic function that is locally Riemann-integrable, where the limit clearly is uniform in $a \in \mathbb{R}$.

Example 6.3.2. Fix $k \in \mathbb{R}$ and consider the trigonometric monomial defined by $\psi_k(x) = \mathrm{e}^{2\pi \mathrm{i} k x}$. Unless $k = 0$, in which case $\psi_0 \equiv 1$, the function ψ_k has period $\frac{1}{|k|} > 0$. For $\alpha \in \mathbb{R}$ with $|\alpha| > 1$, Fact 6.3.1 implies that

$$\frac{1}{N} \sum_{n=0}^{N-1} \psi_k(\alpha^n x) \;\xrightarrow{N\to\infty}\; M(\psi_k) \,=\, \begin{cases} 1, & k = 0, \\ 0, & \text{otherwise,} \end{cases}$$

holds for a.e. $x \in \mathbb{R}$.

More generally, if $(u_n)_{n\in\mathbb{N}_0}$ with $\inf_{n\neq m}|u_n - u_m| > 0$ is the type of sequence from Remark 6.2.4, the above convergence statement also holds with $\alpha^n x$ replaced by $u_n x$. ♢

It is clear from the proof of Fact 6.3.1 that, for periodic functions, it suffices to consider the case $L = 1$ without loss of generality, as we do from now on. Our next step shows that, for $\alpha \in \mathbb{Z}$, one can go beyond the class of 1-periodic functions that are locally Riemann-integrable.

Lemma 6.3.3. *Consider a function $f \in L^1_{\mathrm{loc}}(\mathbb{R})$ that is 1-periodic. Fix some $q \in \mathbb{Z}$ with $|q| \geqslant 2$. Then, for a.e. $x \in \mathbb{R}$, one has*

$$\frac{1}{N}\sum_{n=0}^{N-1} f(q^n x) \xrightarrow{N\to\infty} \int_0^1 f(y)\,\mathrm{d}y \,=\, M(f).$$

Proof. Since $q \in \mathbb{Z}$, we may view the average as a Birkhoff sum for the dynamical system on $[0,1]$ defined by the mapping $x \mapsto qx \bmod 1$. It is well known that Lebesgue measure is invariant and ergodic for this system, compare [11] and references therein, wherefore we may employ Birkhoff's ergodic theorem [37] to f, which is Lebesgue-integrable on $[0,1]$ by assumption, and our claim follows. □

Note that the exceptional set, for which the limit differs or does not exist, may depend on f when the latter fails to be continuous. In fact, there clearly is no uniformly distributed sequence that will work for *all* 1-periodic $f \in L^1_{\mathrm{loc}}(\mathbb{R})$. Still, the result of Lemma 6.3.3 suggests that something more general than Fact 6.3.1 might also be true when our multiplier α fails to be an integer. However, we cannot apply the 'trick' with Birkhoff's ergodic theorem when $\alpha \notin \mathbb{Z}$. This is due to the fact that the sequence $\big(\langle \alpha^n x\rangle\big)_{n\in\mathbb{N}_0}$, which is uniformly distributed on $[0,1)$ for a.e. $x \in \mathbb{R}$ by Fact 6.2.3, does no longer agree with the orbit of x under the mapping T defined by $x \mapsto \alpha x \bmod 1$. The latter, for a.e. $x \in \mathbb{R}$, follows the distribution of the (ergodic) Rényi–Parry measure [31, 29] for α, which is of the form $h_\alpha \lambda$ with h_α being Lebesgue-integrable on $[0,1)$. When $\alpha \notin \mathbb{Z}$, the measures λ and $h_\alpha\lambda$ are still equivalent as measures, but different; see [11] and references therein for more.

Example 6.3.4. To illustrate the difference, let us consider the golden mean $\alpha = \tau = \frac{1}{2}\big(1+\sqrt{5}\,\big)$, which is one of the simplest examples in this context. When f is 1-periodic and locally Riemann-integrable, we get

$$\frac{1}{N}\sum_{n=0}^{N-1} f(\tau^n x) \xrightarrow{N\to\infty} \int_0^1 f(x)\,\mathrm{d}x \,=\, M(f)$$

for a.e. $x \in \mathbb{R}$ by Weyl's criterion (Lemma 6.2.1).

In comparison, let T be defined by $x \mapsto \tau x \bmod 1$ on $[0,1)$. Then, for a.e. $x \in [0,1)$, the orbits $(T^n x)_{n\in\mathbb{N}_0}$ follow the distribution given by the piecewise constant function [31, Ex. 4]

$$h_\tau(x) \,=\, \begin{cases} \frac{5+3\sqrt{5}}{10}, & 0 \leqslant x < \frac{1}{\tau}, \\ \frac{5+\sqrt{5}}{10}, & \frac{1}{\tau} \leqslant x < 1. \end{cases}$$

Since T is ergodic for the measure $h_\tau\lambda$, Birkhoff's theorem tells us that, for any Lebesgue-integrable function f on $[0,1)$, one has

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x) \,=\, \int_0^1 f(x)\, h_\tau(x)\, \mathrm{d}x$$

for a.e. $x \in [0,1)$, and this limit will generally differ from $M(f)$.

Moreover, since the sequences $(\langle \tau^n x\rangle)_{n\geqslant 0}$ and $(T^n x)_{n\geqslant 0}$ are not easily relatable, one cannot infer the convergence of averages along the exponential sequence from those along the orbits under T. $\Diamond$

Let us now extend Fact 6.3.1 beyond Riemann-integrable functions by stating one version of Sobol's theorem [33, Thm. 1].

Theorem 6.3.5. *Let $\alpha \in \mathbb{R}$ with $|\alpha| > 1$ be fixed, and consider a 1-periodic function $f \in L^1_{\mathrm{loc}}(\mathbb{R})$ that fails to be locally Riemann-integrable. Assume that there is a finite set $F \subset [0,1]$ such that f, for every $\delta > 0$, is Riemann-integrable on the complement of $F+(-\delta,\delta)$ in $[0,1]$. Assume further that, for every $z \in F$, there is a $\delta_z > 0$ such that f is differentiable on the punctured interval $(z-\delta_z, z+\delta_z)\setminus\{z\}$ and that, for any $s > 0$,*

$$V_N(z,s) \,:=\, \int_{z-\delta_z}^{z-\frac{1}{N^s}} |f'(x)|\,\mathrm{d}x \,+\, \int_{z+\frac{1}{N^s}}^{z+\delta_z} |f'(x)|\,\mathrm{d}x \,=\, \mathcal{O}\big(N^{\frac{s}{2}-\eta}\big)$$

holds for some $\eta = \eta(z) > 0$ as $N \to \infty$.

Then, for a.e. $x \in \mathbb{R}$, one has

$$\frac{1}{N} \sum_{n=0}^{N-1} f(\alpha^n x) \,\xrightarrow{N\to\infty}\, \int_0^1 f(y)\,\mathrm{d}y \,=\, M(f).$$

Sketch of proof. Since F is finite, we may choose $0 < \delta \leqslant \min_{z\in F} \delta_z$ small enough such that the open sets $(z-\delta, z+\delta)$ with $z \in F$ are disjoint. By writing f as a sum of a locally Riemann-integrable function (such as the restriction $f^{(\delta)}$ of f to the complement of $\mathbb{Z}+F+(-\delta,\delta)$) and $r = \mathrm{card}(F)$ 'problematic' terms, the latter supported on $\mathbb{Z}+(z-\delta, z+\delta)$ with $z \in F$, it is clear that our claim follows if we can deal with one of these problematic terms. So, select one $z \in F$. Without loss of generality, we may assume that $(z-\delta, z+\delta) \subset [0,1]$, as we can otherwise shift the unit interval because f and $f^{(\delta)}$ are 1-periodic.

One can now repeat the original proof from [33], or the more extensive version in [20, Sec. 2]. Here, the validity of the convergence claim emerges from the observation that, for a.e. $x \in \mathbb{R}$, the number $\langle \alpha^{n-1} x \rangle$ does not come closer to z than $1/n^{1+\varepsilon}$, for any fixed $\varepsilon > 0$ and then all $n \in \mathbb{N}$ except at most finitely many. This follows from Lemma 6.2.6 with $Y = z + \mathbb{Z}$. Now,

$$V_N(z, 1+\varepsilon) \,=\, o\Big(N^{\frac{1+\varepsilon}{2}-\eta}\Big)$$

for some $\eta > 0$ by assumption. Since η does not depend on ε, we are still free to choose $\varepsilon > 0$ small enough so that $\vartheta := \eta - \frac{\varepsilon}{2} > 0$.

Now, the potentially large contributions to our averaging sum from sequence elements close to z are properly 'counterbalanced' by the discrepancy of $(\alpha^n x)_{n\in\mathbb{N}}$, where we invoke Fact 6.2.5 with the ε just chosen. One obtains

$$\mathcal{D}_N \cdot V_N(z, 1+\varepsilon) \,=\, o\Big(\frac{\big(\log(N)\big)^{\frac{3}{2}+\varepsilon}}{N^{\vartheta}}\Big) \,=\, o(1), \tag{6.3.1}$$

which is a sufficient criterion for the claimed convergence because

$$\frac{1}{N}\sum_{n=0}^{N-1} f^{(\delta)}(\alpha^n x) \;\xrightarrow{N\to\infty}\; M\big(f^{(\delta)}\big)$$

holds for a.e. $x \in \mathbb{R}$, while the Birkhoff average of $f - f^{(\delta)}$ is controlled by Eq. (6.3.1) and tends to 0 as $\delta \searrow 0$. □

Remark 6.3.6. The assumption that F in Theorem 6.3.5 is a finite set implies that $\delta := \min_{z\in F} \delta_z > 0$ as well as $\min_{z\in F} \eta(z) > 0$. Later, we will replace this setting by a suitable compactness assumption to extend the result of this theorem to almost periodic functions. ♢

Remark 6.3.7. The differentiability assumption for f near the 'bad' points is convenient, but not necessary. It can be replaced by the requirement that the total variation of f on sets of the form $(z-\delta, z-N^{-s}] \cup [z+N^{-s}, z+\delta)$ behaves as stated for $V_N(z,s)$; compare [33, 20]. ♢

As mentioned earlier, results of this type are also of interest for the numerical calculation of integrals, for instance with methods of (quasi-) Monte Carlo type [25]. In our context, an important question is how to extend Riesz–Raikov sums and Birkhoff averages to functions that fail to be periodic, but possess some repetitivity structure instead.

6.4. Averaging almost periodic functions

At this point, we need to recall some basic definitions and results from the theory of almost periodic functions in the sense of Bohr [8], where we refer to

[AO1, Sec. 8.2] for a short summary, to [23, Sec. VI.5] or [13] for comprehensive expositions, and to [27, Sec. 41] for a more general and abstract setting (including non-Abelian groups).

Recall that $f \in C(\mathbb{R})$ is called *almost periodic in the sense of Bohr* if, for any $\varepsilon > 0$, the set of ε-almost periods

$$\mathcal{P}_\varepsilon := \bigl\{t \in \mathbb{R} : \|f - T_t f\|_\infty < \varepsilon\bigr\}$$

is relatively dense in $\mathbb{R}$. Here, $\bigl(T_t f\bigr)(x) := f(x-t)$ defines the t-translate of f. Any continuous periodic function is almost periodic in this sense, as is any trigonometric polynomial. Any Bohr-almost periodic function is bounded and uniformly continuous. In fact, the $\|.\|_\infty$-closure of the (complex) algebra of trigonometric polynomials is precisely the space of *all* Bohr-almost periodic functions [8].

For comparison, $f \in C(\mathbb{R})$ is called *almost periodic in the sense of Bochner* (for $\|.\|_\infty$, to be precise) if the translation orbit $\{T_t f : t \in \mathbb{R}\}$ is precompact in the $\|.\|_\infty$-topology. The fundamental relation among these notions can be summarised as follows; see [AO1, Prop. 8.2] as well as [23, 13].

Fact 6.4.1. *For $f \in C(\mathbb{R})$, the following properties are equivalent.*

(1) *f is Bohr-almost periodic, i.e., $\mathcal{P}_\varepsilon$ is relatively dense for any $\varepsilon > 0$;*
(2) *f is Bochner-almost periodic for $\|.\|_\infty$, i.e., the orbit $\{T_t f : t \in \mathbb{R}\}$ is precompact in the $\|.\|_\infty$-topology;*
(3) *f is the limit of a sequence of trigonometric polynomials, with uniform convergence of the sequence on $\mathbb{R}$.* □

In view of these relations, we follow [5] and speak of *uniformly almost periodic functions* from now on when we refer to this class. If misunderstandings are unlikely, we will drop the attribute 'uniformly'. Let us elaborate a little on part (3) of Fact 6.4.1. If f is almost periodic, its mean

$$M(f) = \lim_{T\to\infty} \frac{1}{2T} \int_{a-T}^{a+T} f(x)\,\mathrm{d}x \tag{6.4.1}$$

exists for any $a \in \mathbb{R}$, is independent of a, and the convergence is uniform in a; compare Definition 4.1.6 and the discussion of this concept in Chapter 4. When we need to emphasise the role of a for more general types of functions (say without uniformity of the limit in a), we will write $M(f;a)$.

The *Fourier–Bohr coefficient* of an almost periodic function f at $k \in \mathbb{R}$ is given by

$$a(k) = M\bigl(\mathrm{e}^{-2\pi \mathrm{i} k(.)} f\bigr).$$

It exists for any $k \in \mathbb{R}$, and differs from 0 for at most countably many values of k. Any $k \in \mathbb{R}$ with $a(k) \neq 0$ is called a *frequency* of f. If $\{k_\ell\}$ is the set of

frequencies of f, there is a sequence of trigonometric polynomials of the form

$$P^{(m)}(x) = \sum_{\ell=1}^{n_m} r_\ell^{(m)}\, a(k_\ell)\, \mathrm{e}^{2\pi \mathrm{i} k_\ell x} \tag{6.4.2}$$

that converge uniformly to f on $\mathbb{R}$ as $m \to \infty$. Here, the numbers $r_\ell^{(m)}$, which are known as convergence enforcing numbers, depend on m and k_ℓ, but not on $a(k_\ell)$, and can be chosen as rational numbers [13, Thm. I.1.24].

To approach averages of almost periodic functions, it is thus more than natural to begin with the averages of trigonometric polynomials. We formulate the next result for more general sequences than the exponential ones from above.

Proposition 6.4.2. *Let P_m be a (complex) trigonometric polynomial of the form $P_m(x) = a_0 + \sum_{\ell=1}^{m} a_\ell\, \mathrm{e}^{2\pi \mathrm{i} k_\ell x}$, with complex coefficients a_ℓ and distinct non-zero frequencies $k_1, \ldots, k_m$. Further, let $(u_n)_{n\in\mathbb{N}_0}$ be a sequence of real numbers such that $\inf_{n\neq m} |u_n - u_m| > 0$. Then, for a.e. $x \in \mathbb{R}$, one has*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} P_m(u_n x) \,=\, M(P_m) \,=\, a_0 .$$

In particular, this holds for $u_n = \alpha^n$ with $\alpha \in \mathbb{R}$ and $|\alpha| > 1$.

Proof. The claim is obvious for $m = 0$, where the polynomial is constant. The case $m = 1$ with $a_0 = 0$, where P_m is a monomial, is Example 6.3.2 from above. So, for a general P_m, the claim is true for each summand individually, with an exceptional set $E(k_\ell)$ of measure 0 for $\ell \geqslant 1$. Since $\bigcup_{\ell=1}^{m} E(k_\ell)$ is still a null set, the statement on the limit is clear, while its value follows from a simple calculation with the mean; compare Example 6.3.2. □

Before we proceed, let us recall the following useful property of the mean.

Lemma 6.4.3. *Let $(g_n)_{n\in\mathbb{N}}$ be a sequence of complex-valued, but not necessarily continuous, functions on $\mathbb{R}$ that converge uniformly to a function f. Assume further that the mean $M(g_n)$ exists for all $n \in \mathbb{N}$. Then, also $M(f)$ exists, and $\lim_{n\to\infty} M(g_n) = M(f)$. In particular, one has*

$$M(f) \,=\, \lim_{T\to\infty} \frac{1}{2T} \int_{a-T}^{a+T} f(x)\, \mathrm{d}x$$

for any fixed $a \in \mathbb{R}$. When the convergence of the means $M(g_n) = M(g_n; a)$ is uniform in a, then so is the convergence of $M(f)$.

Proof. The assumed uniform convergence also means that $(g_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in the $\|.\|_\infty$-topology. Fix $\varepsilon > 0$ and choose $n_0 = n_0(\varepsilon)$ such that $\|g_n - f\|_\infty < \varepsilon$ as well as $\|g_n - g_m\|_\infty < \varepsilon$ holds for all $n, m \geqslant n_0$.

Then, for any $T > 0$, one has

$$\frac{1}{2T}\left|\int_{-T}^{T}\bigl(g_n(x)-g_m(x)\bigr)\,\mathrm{d}x\right| \leqslant \bigl\|g_n-g_m\bigr\|_\infty < \varepsilon \tag{6.4.3}$$

for all $n, m \geqslant n_0$, which implies

$$\begin{aligned}\bigl|M(g_n)-M(g_m)\bigr| &\leqslant \bigl\|g_n-g_m\bigr\|_\infty \\ &\quad + \left|M(g_n)-\frac{1}{2T}\int_{-T}^{T} g_n(x)\,\mathrm{d}x\right| + \left|M(g_m)-\frac{1}{2T}\int_{-T}^{T} g_m(x)\,\mathrm{d}x\right|.\end{aligned}$$

Consequently, $\bigl|M(g_n)-M(g_m)\bigr| < 3\varepsilon$ for all sufficiently large T due to our assumption on the existence of the means $M(g_n)$. Note that, although T may depend on m and n, the 3ε-estimate still works as a consequence of Eq. (6.4.3). The sequence $\bigl(M(g_n)\bigr)_{n\in\mathbb{N}}$ is thus Cauchy, hence convergent, with limit $\mathfrak{M}$, say.

Now, choose $n \geqslant n_0$ large enough such that also $|M(g_n)-\mathfrak{M}| < \varepsilon$ holds, fix an arbitrary $a \in \mathbb{R}$, and consider

$$\begin{aligned}\left|\frac{1}{2T}\int_{a-T}^{a+T} f(x)\,\mathrm{d}x-\mathfrak{M}\right| &\leqslant \bigl\|f-g_n\bigr\|_\infty + \bigl|M(g_n)-\mathfrak{M}\bigr| \\ &\quad + \left|\frac{1}{2T}\int_{a-T}^{a+T} g_n(x)\,\mathrm{d}x - M(g_n)\right| < 3\varepsilon,\end{aligned}$$

where the last step holds for all sufficiently large T by assumption. This derivation implies

$$\lim_{T\to\infty}\frac{1}{2T}\int_{a-T}^{a+T} f(x)\,\mathrm{d}x = \mathfrak{M} = \lim_{n\to\infty} M(g_n),$$

which is independent of $a \in \mathbb{R}$, and $M(f) = \mathfrak{M}$ is the claimed mean of f.

When, in addition, the means of the functions g_n exist uniformly in a, our above 3ε-argument also implies that the convergence of $M(f;a)$ is uniform in $a \in \mathbb{R}$ as claimed. □

This enables us to formulate the following result.

Theorem 6.4.4. *Let $\alpha \in \mathbb{R}$ with $|\alpha| > 1$ be given, and let f be a uniformly almost periodic function on $\mathbb{R}$. Then, for a.e. $x \in \mathbb{R}$, one has*

$$\lim_{N\to\infty}\frac{1}{N}\sum_{n=0}^{N-1} f(\alpha^n x) = M(f).$$

Proof. Let $(g_n)_{n\in\mathbb{N}}$ be a sequence of trigonometric polynomials that converge uniformly to f. As is well known, compare [13], and is a rather direct

consequence of Eq. (6.4.2), the sequence can be chosen such that the frequency sets $\{k_j : 1 \leqslant j \leqslant m_n\}$ of the g_n are nested. By Proposition 6.4.2, we know that, for every $n \in \mathbb{N}$,

$$\lim_{N\to\infty} \frac{1}{N} \sum_{\ell=0}^{N-1} g_n(\alpha^\ell x) \,=\, M(g_n)$$

holds for a.e. $x \in \mathbb{R}$, where we denote the excluded null set by E_n. By construction, we have $E_n \subseteq E_{n+1}$, and $E := \bigcup_{n\in\mathbb{N}} E_n$ is still a null set.

Define the Birkhoff average of φ at x as $S_N(\varphi, x) = \frac{1}{N}\sum_{n=0}^{N-1} \varphi(\alpha^n x)$, and fix some $\varepsilon > 0$. Choose $n_0 = n_0(\varepsilon)$ such that $\|f - g_n\|_\infty < \varepsilon$ for all $n \geqslant n_0$, which is possible under our assumptions. Now, for any fixed $x \in \mathbb{R} \setminus E$, we can estimate

$$\bigl|S_N(f,x) - M(f)\bigr| \,\leqslant\, \bigl|S_N(f-g_n,x)\bigr| + \bigl|S_N(g_n,x) - M(g_n)\bigr| + \bigl|M(g_n) - M(f)\bigr|$$

where, independently of N,

$$\bigl|S_N(f-g_n,x)\bigr| \,\leqslant\, S_N\bigl(|f-g_n|,x\bigr) \,\leqslant\, \|f-g_n\|_\infty \,<\, \varepsilon$$

for any $n \geqslant n_0$. The third term on the right-hand side of the previous estimate is smaller than ε for sufficiently large n as a consequence of Lemma 6.4.3, while the middle term, under our assumptions, is bounded by ε for sufficiently large N, which we are still free to choose. This 3ε-argument thus establishes the claim. □

Let us mention in passing that Theorem 6.4.4 still holds if α^n, as before, is replaced by the numbers u_n of a sequence as described in Remark 6.2.4.

At this point, to go any further, we need to extend the class of functions we consider. This is motivated by the fact that uniform almost periodicity is often too restrictive. In particular, in various examples from dynamical systems theory, one encounters averages over functions that fail to be bounded, and hence cannot be uniformly almost periodic. Being unbounded, such functions cannot be locally Riemann-integrable either, though they might still admit improper Riemann integrals or be locally Lebesgue-integrable.

It would be natural to investigate the question in the setting of weakly almost periodic functions, as introduced in Chapter 4, which seems possible as well. However, the above remarks indicate that one needs results also for functions that violate continuity. This suggests to use the wider class of almost periodic functions in the sense of Stepanov[3] [34], which relate to

[3]The widely used modern version of the name is V.V. Stepanov, while the author used W. Stepanoff in his original articles.

locally Lebesgue-integrable functions like uniformly almost periodic functions do to continous functions. The new norm on $L^1_{\mathrm{loc}}(\mathbb{R})$ is given by

$$\|f\|_{\mathrm{S}} = \sup_{x\in\mathbb{R}} \frac{1}{L} \int_x^{x+L} |f(y)|\,\mathrm{d}y,$$

where $L > 0$ is an arbitrary, but fixed number. Since these norms are equivalent for different values of L, it is most convenient to choose $L = 1$, as we do from now on. Now, a locally Lebesgue-integrable function f is called *almost periodic in the sense of Stepanov*, or S-almost periodic for short, if, for any $\varepsilon > 0$, the set $\mathcal{P}^{\mathrm{S}}_{\varepsilon}$ of ε-almost periods of f for $\|.\|_{\mathrm{S}}$ is relatively dense. The analogue of Fact 6.4.1 then reads as follows (we omit a proof because it works the same way as in the previous case; compare [13]).

Fact 6.4.5. *For $f \in L^1_{\mathrm{loc}}(\mathbb{R})$, the following properties are equivalent.*

(1) *f is S-almost periodic, i.e., $\mathcal{P}^{\mathrm{S}}_{\varepsilon}$ is relatively dense for any $\varepsilon > 0$;*
(2) *f is Bochner-almost periodic for $\|.\|_{\mathrm{S}}$, i.e., the orbit $\{T_t f : t \in \mathbb{R}\}$ is precompact in the $\|.\|_{\mathrm{S}}$-topology;*
(3) *f is the $\|.\|_{\mathrm{S}}$-limit of a sequence of trigonometric polynomials.* □

Let us note in passing that every locally integrable function f on $\mathbb{R}$ may be viewed as a translation bounded measure (where f is the Radon–Nikodym density relative to λ). In doing so, the Stepanov norm is induced by the $\|.\|_{[0,1]}$-norm for measures as discussed in Chapter 5. This implies that a function $f \in L^1_{\mathrm{loc}}(\mathbb{R})$ is S-almost periodic if and only if the measure $f\lambda$ is norm-almost periodic in the sense of Definition 5.3.1; see also [4].

Every uniformly almost periodic function is S-almost periodic, which also means (via part (3) of Fact 6.4.5) that any S-almost periodic function can be $\|.\|_{\mathrm{S}}$-approximated by uniformly almost periodic functions. In other words, the class of all S-almost periodic functions can equivalently be described as the $\|.\|_{\mathrm{S}}$-closure of the (complex) algebra of trigonometric polynomials or as that of the class of uniformly almost periodic functions. Moreover, the space of S-almost periodic functions is complete in the $\|.\|_{\mathrm{S}}$-norm, and $\|f\|_{\mathrm{S}} = 0$ means $f = 0$ in the Lebesgue sense, so $f(x) = 0$ for a.e. $x \in \mathbb{R}$; see [6] for details.

Remark 6.4.6. If f is S-almost periodic, its mean exists. In fact, observe that, for all S-almost periodic functions f, g and for any $a \in \mathbb{R}$, one has

$$\frac{1}{2T}\left|\int_{a-T}^{a+T} \bigl(f(x) - g(x)\bigr)\,\mathrm{d}x\right| \leqslant \frac{1+[2T]}{2T}\,\bigl\|f-g\bigr\|_{\mathrm{S}}.$$

Now, it is immediate that the statement of Lemma 6.4.3 still holds if uniform convergence is replaced by $\|.\|_{\mathrm{S}}$-convergence. This then gives the desired existence of means because, by Fact 6.4.5(3), we can $\|.\|_{\mathrm{S}}$-approximate

any S-almost periodic function with trigonometric polynomials for which the mean clearly exists. ◊

As an aside, we mention the following interesting connection.

Lemma 6.4.7. *Let f be an* S*-almost periodic function, and let $\delta > 0$ be arbitrary, but fixed. Then, the function f_δ defined by*

$$f_\delta(x) \,=\, \frac{1}{2\delta}\int_{x-\delta}^{x+\delta} f(y)\,\mathrm{d}y$$

is continuous and uniformly almost periodic. Moreover, $\lim_{\delta\searrow 0} f_\delta = f$ in the $\|.\|_{\mathrm{S}}$-topology.

Proof. Assume $\delta \leqslant \frac{1}{2}$ (the argument for $\delta > \frac{1}{2}$ is analogous), and let t be a $(2\delta\varepsilon)$-almost period of f for $\|.\|_{\mathrm{S}}$. Now,

$$\begin{aligned}\bigl|f_\delta(t+x) - f_\delta(x)\bigr| \,&=\, \frac{1}{2\delta}\left|\int_{x-\delta}^{x+\delta} f(t+y) - f(y)\,\mathrm{d}y\right| \\ &\leqslant\, \frac{1}{2\delta}\int_{x-\delta}^{x-\delta+1}\bigl|f(t+y)-f(y)\bigr|\,\mathrm{d}y \,\leqslant\, \frac{\|f - T_t f\|_{\mathrm{S}}}{2\delta} \,<\, \varepsilon\end{aligned}$$

which implies that t is an ε-almost period of f_δ for $\|.\|_\infty$. Via part (1) of Fact 6.4.5, we conclude that f_δ satisfies part (1) of Fact 6.4.1, and thus is uniformly almost periodic. As such, f_δ is also uniformly continuous.

For the second claim, we refer to the original proof in [6], which uses an approximation argument that is based on the effect that a 'convolution mollifier' has on a locally Lebesgue-integrable function. □

The main extension of Theorem 6.3.5 can be stated as follows.

Theorem 6.4.8. *Let $\alpha \in \mathbb{R}$ with $|\alpha| > 1$ be fixed, and let $f \in L^1_{\mathrm{loc}}(\mathbb{R})$ be an* S*-almost periodic function. Assume now that there is a uniformly discrete set $Y \subset \mathbb{R}$ such that f, for every $\delta > 0$, is locally Riemann-integrable on the complement of $Y + (-\delta, \delta)$. Assume further that there is a $\delta' > 0$ such that, for any $z \in Y$, f is differentiable on the punctured interval $(z-\delta', z+\delta')\setminus\{z\}$ and that, for any $s > 0$ and with $V_N(z,s)$ as defined in Theorem* 6.3.5*,*

$$\sup_{z\in Y} V_N(z,s) \,=\, o\bigl(N^{\frac{s}{2}-\eta}\bigr)$$

holds for some $\eta > 0$ as $N \to \infty$.

Then, for a.e. $x \in \mathbb{R}$, one has

$$\lim_{N\to\infty}\frac{1}{N}\sum_{n=0}^{N-1} f(\alpha^n x) \,=\, M(f),$$

where the mean exists because f is S*-almost periodic.*

Sketch of proof. Without loss of generality, we may assume that δ' is small enough so that the open intervals $(z-\delta', z+\delta')$ with $z \in Y$ are disjoint. Now, Lemma 6.2.6 guarantees that the sequence $(\alpha^{n-1}x)_{n\in\mathbb{N}}$, for a.e. $x \in \mathbb{R}$, does not come closer to Y than $1/n^{1+\varepsilon}$, for any fixed $\varepsilon > 0$ and then for all $n \in \mathbb{N}$ except at most finitely many.

For any $z \in Y$, we have $V_N(z, 1+\varepsilon) = o\big(N^{\frac{1+\varepsilon}{2}-\eta}\big)$ for some fixed $\eta > 0$ by assumption, where we may once again assume that $\varepsilon > 0$ is chosen such that $\vartheta = \eta - \frac{\varepsilon}{2} > 0$. With the estimate of Eq. (6.3.1) in the proof of Theorem 6.3.5, we again obtain $\mathcal{D}_N \cdot V_N(z, 1+\varepsilon) = o(1)$ as $N \to \infty$, which establishes a sufficient criterion for the claimed convergence.

Indeed, let $0 < \delta < \delta'$ be arbitrary, and let 1_δ denote the characteristic function of the set $\mathbb{R} \setminus \big(Y + (-\delta, \delta)\big)$. Obviously, for any such δ, the function $f^{(\delta)} := f \cdot 1_\delta$ is both S-almost periodic and locally Riemann-integrable on $\mathbb{R}$. For a.e. $x \in \mathbb{R}$, we thus get

$$\frac{1}{N}\sum_{n=0}^{N-1} f^{(\delta)}(\alpha^n x) \xrightarrow{N\to\infty} M\big(f^{(\delta)}\big) \xrightarrow{\delta\searrow 0} M(f)$$

by a combination of our previous arguments. Since the average of $f - f^{(\delta)}$ along the exponential sequence is controlled by the above mentioned estimate from Eq. (6.3.1), our claim follows. □

Note that our assumption on η achieves the analogue of the comment made in Remark 6.3.6. Note also that Remark 6.3.7 has an obvious extension to this more general situation. Indeed, one can once again replace the differentiability condition by the corresponding behaviour of the total variation in the vicinity of the 'bad' points.

6.5. Further directions and extensions

Our exposition so far used complex-valued almost periodic functions over $\mathbb{R}$, mainly for ease of presentation. More generally, one is interested in vector-valued functions, or in function with values in an arbitrary Banach space $\mathbb{X}$, with norm $|.|$ say. So, let $f : \mathbb{R} \longrightarrow \mathbb{X}$ be such a function, and define $\|f\|_\infty = \sup_{x\in\mathbb{R}} |f(x)|$. Then, the ε-almost periods of f are again defined as

$$\mathcal{P}_\varepsilon := \{t \in \mathbb{R} : \|f - T_t f\|_\infty < \varepsilon\},$$

with $\big(T_t f\big)(x) = f(x-t)$ as before.

Likewise, one can define trigonometric polynomials (or functions), by which one now means any function $T\colon \mathbb{R} \longrightarrow \mathbb{X}$ of the form

$$Q_m(x) \;=\; a_0 \,+\, \sum_{\ell=1}^{m} \mathrm{e}^{2\pi \mathrm{i} k_\ell x}\, a_\ell \tag{6.5.1}$$

for some $m \geqslant 0$, where $\{k_1, \ldots, k_\ell\}$ are distinct, non-zero real numbers and where the a_ℓ are now elements of $\mathbb{X}$. When $m = 0$, the sum is meant to be empty and Q_m is constant. The analogue of Fact 6.4.1 can now be stated as follows; see [13, Ch. VI] for details.

Fact 6.5.1. *Let $(\mathbb{X}, |.|)$ be a Banach space. Then, for a continuous function $f\colon \mathbb{R} \longrightarrow \mathbb{X}$, the following properties are equivalent.*

(1) *f is Bohr-almost periodic, i.e., $\mathcal{P}_\varepsilon$ is relatively dense for any $\varepsilon > 0$;*
(2) *f is Bochner-almost periodic for $\|.\|_\infty$, i.e., the orbit $\{T_t f : t \in \mathbb{R}\}$ is precompact in the $\|.\|_\infty$-topology;*
(3) *f is the limit of a sequence of trigonometric polynomials, with uniform convergence of the sequence on $\mathbb{R}$.* □

There is no surprise up to this point, and we have gained rather little. As before, we call such functions uniformly almost periodic. To continue, we need the notion of the *mean* of such a function f, and also some generalisation of the Fourier series expansions. For this, we have to be able to (locally) integrate the function f. A natural approach is provided by *Bochner's integral* [7], which can be viewed as an extension of the Lebesgue integral to functions with values in a general Banach space; see [12, App. E] or [39, Sec. V.5] for modern expositions.

With this extension, most of our previous results remain true, with the only change that the coefficients a_ℓ are now elements of $\mathbb{X}$ rather than complex numbers. For instance, one has $M(Q_m) = a_0$ for the trigonometric polynomial of Eq. (6.5.1), and the analogue of Proposition 6.4.2 holds without change. Now, also the consecutive steps have their natural analogues, and we obtain the following result.

Theorem 6.5.2. *Let $(\mathbb{X}, |.|)$ be a Banach space, and let $f : \mathbb{R} \longrightarrow \mathbb{X}$ be uniformly almost periodic. Then, for any fixed $\alpha \in \mathbb{R}$ with $|\alpha| > 1$, one has*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} f(\alpha^n x) \,=\, M(f),$$

which holds for a.e. $x \in \mathbb{R}$. □

The extension to almost periodic functions in the Stepanov sense works in complete analogy, and we leave further steps in this direction to the reader.

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EPILOGUE

Gateways Towards Quasicrystals

Peter Kramer

The experimental discovery of quasicrystals by Shechtman, Gratias, Blech and Cahn [44] provided the paradigm for a new type of long-range order of solid matter in Nature. This discovery stimulated an explosion of new experimental and theoretical research. Prior to the discovery, however, there was already an active development of various gateways to quasicrystals in theoretical and mathematical physics. Without this conceptual basis, it would have been impossible to grasp and to efficiently explore the structure and physical properties of quasicrystrals. The aim of this overview is to give a non-technical and condensed account of the conceptual gateways to quasicrystals prior to their discovery.

E.1. Classical periodic crystallography

A. Bravais, J.B.J. Fourier, A.M. Schönflies and E.S. Fedorov

Crystals in the natural world have long been the subject of widespread attention due to their regular geometric, polyhedral form. It was A. Bravais [3] who obtained fundamental insight into their internal structure by introducing the idea of an underlying periodic lattice Γ; see Figure E.1.1. Bravais was able to explain the regularity of crystal facets by associating them with planes uniformly occupied by lattice points. The finite translations that connect lattice points form the translation group of the lattice, also denoted by Γ for short. If the neighbouring distances and directions in a lattice are tuned in particular ways, finite rotations with respect to a fixed lattice point may move lattice points to lattice points. The lattice then is compatible with a *point group*.

Consideration of the combined symmetries under lattice translations and rotations led to the concept of *space group* symmetries. The question then arose: What are the possible crystal structures in three-dimensional space? Exploration of this question in the 19th century culminated in the systematic classification of all possible crystal structures in terms of space group theory

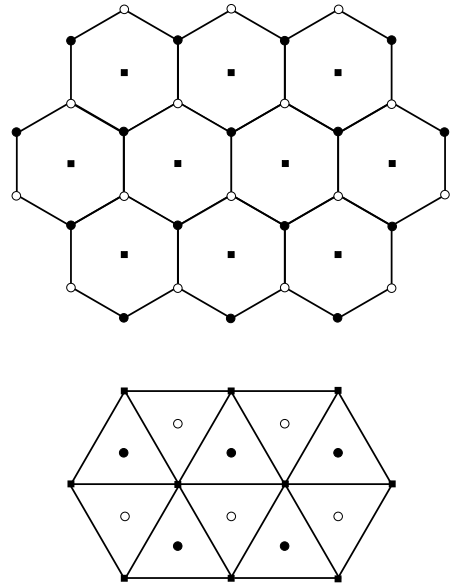

FIGURE E.1.1. Hexagonal packing and dual triangular periodic lattice. The centres (white and black circles) of the dual triangular cells are located at the vertices of the hexagonal cells (centres black squares). The hexagons and triangles are examples of the Voronoi and dual Delone cells in general periodic lattices; compare [29] as well as [AO1, Sec. 2.2].

by Schönflies [41, 42] and Fedorov [7]. The emergence of an atomic structure model of solid matter in the 19th century offered the possibility of viewing a crystal lattice as being formed by atoms. The atomic structure was verified in 1912 in diffraction experiments with X-rays following von Laue and Bragg; see [11, Ch. 1].

The concept of a periodic lattice implies other basic notions for crystals: The periodic lattice symmetry ensures that the long-range distribution of atoms is completely determined once it is known inside a unit cell. The analysis of periodic systems was fundamentally advanced by Fourier's concept [8] of the series expansion of a periodic function into elementary periodic functions. For a complex-valued periodic function $f^{\mathsf{p}}(x)$ (with period 1) on the real line, this expansion, in a condensed complex version, takes the form

$$\begin{aligned} f^{\mathsf{p}}(x) &= \sum_{\mu\in\mathbb{Z}} a(k_\mu)\exp(\mathrm{i}k_\mu x), \quad \text{with } k_\mu := 2\pi\mu \text{ for } \mu\in\mathbb{Z}, \\ a(k_\mu) &= \int_{-1/2}^{1/2} \exp(-\mathrm{i}k_\mu x) f^{\mathsf{p}}(x)\,\mathrm{d}x. \end{aligned} \tag{E.1.1}$$

The Fourier coefficients $a(k_\mu)$ in this expansion, given as integrals of the function $f^{\mathsf{p}}(x)$ over the unit interval, may be considered as values of a function defined on the points k_μ of a lattice Γ^{R} in Fourier k-space. Thus, the Fourier series represents the function f^{p}, with the unit interval as its domain, via a function on the points of the so-called reciprocal lattice Γ^{R} in k-space, where $\Gamma^{\mathsf{R}} = 2\pi\Gamma^*$ with the dual lattice Γ^* as defined in [AO1, Eq. (3.4)]. Similarly, for crystals with lattices in 3-space $\mathbb{E}^3$, the Fourier coefficients live on a three-dimensional k-space that is equipped with a three-dimensional reciprocal lattice Γ^{R}.

With the advent of scattering theory via quantum wave mechanics, von Laue and Bragg [11] directly related the magnitude of the Fourier coefficients to the observed intensity of waves scattered from crystals. The scattering intensity from crystals is characterised by sharp peaks in selected directions. In mathematical terms, one speaks of a Fourier point spectrum; compare [AO1, Ch. 9]. To date, the determination of the atomic structure of matter is based on the interpretation of scattering data by Fourier series and, more generally, by Fourier analysis.

The three related notions of a periodic lattice Γ, an atomic unit cell and a Fourier series analysis characterise crystals as atomic structures with periodic long-range order.

E.2. Point symmetry: Das Pentagramma macht Dir Pein?

Another geometric aspect of crystals observed in Nature was the presence of regular angles between their outer facets. With respect to the centre of the crystal, these facets often displayed twofold, fourfold or sixfold point symmetry as part of their polyhedral symmetry. These properties found an explanation in terms of Bravais' periodic lattice theory: It was shown that all the observed point symmetries could be related to what became known as the 14 Bravais lattices, grouped into seven lattice systems. The compatibility of point and periodic lattice symmetry in the framework of space groups formed the basis of the classification by Schönflies and Fedorov.

Yet, there remained an enigma expressed by J.W. von Goethe in his drama Faust [46]: *Das Pentagramma macht Dir Pein?* Certain well-known point symmetries did not fit into lattice theory of two- or three-dimensional space. Among them were the fivefold and the icosahedral symmetries, associated with the cyclic group C_5 (in two or three dimensions) and the icosahedral group Y of rotations in three dimensions; compare [AO1, Sec. 3.2] and references therein for background. Two thousand years earlier, in his study of regular polyhedra, Plato [40] had already noted the regular dodecahedron and icosahedron with icosahedral symmetry. For him, four regular polyhedra

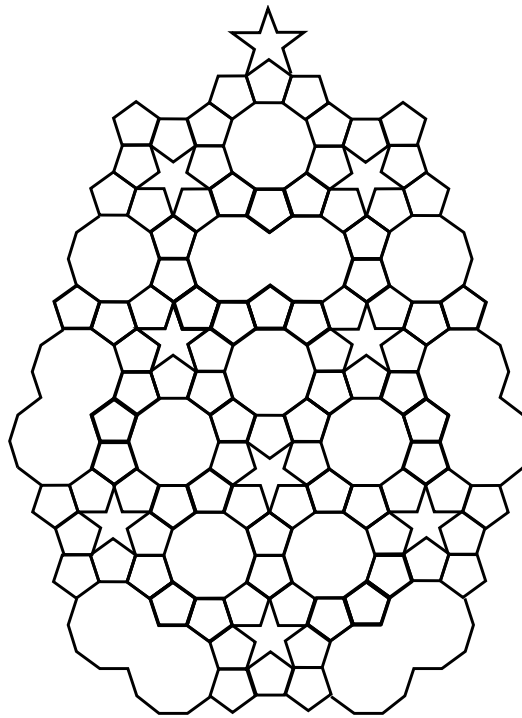

FIGURE E.2.1. Kepler's planar tiling patch with decagons and pentagons. He found that, in order to leave no gaps, he needed pentagons and pentagonal stars in addition to decagons.

were geometric building blocks of the four elements, whereas he associated the dodecahedron with the overall symmetry.

J. Kepler [19] was impressed by the Platonic catalogue. In a first attempt, he tried to use the polyhedra to determine the radii of planetary spheres. Later, after his discovery of the elliptic orbits of the planets, he studied [20] regular polygons and polyhedra in order to deduce rational relationships between astronomical data for the orbits of the planets. In his studies, he also looked at tilings of the plane by regular pentagons, see Figure E.2.1, and enlarged the list of polyhedra by the semi-regular triacontahedron.

With the success of crystallographic lattice theory in the 19th century and its subsequent atomic setting via quantum theory, fivefold and icosahedral point symmetry, being incompatible with any two- or three-dimensional lattice, were stigmatised as being *non-crystallographic*. Of course, fivefold and icosahedral point symmetry can and do appear in molecules. But all the known paradigms of long-range order were thought to be periodic, and hence lattice-based, and thus excluded these point symmetries.

In view of their geometric realisability in three-dimensional space (in terms of group representation theory) the enigma remained: Are these point symmetries simply forbidden in Nature, since they are not compatible with any lattice, or can they be the gateways towards a new type of long-range order in Nature?

E.3. Mathematical crystallography in higher dimensions

H. Zassenhaus and C. Hermann 1948/49

The determination of all space groups in three-dimensional Euclidean space was an obvious classification problem in mathematical physics, with a clear counterpart in Euclidean spaces of higher dimension. The systematic analysis of these symmetries and lattices was advanced in particular by H. Zassenhaus [49] and by C. Hermann [12]. Their work, reviewed by Schwarzenberger [43], showed that the counterparts of all essential findings of classical crystallography in $\mathbb{E}^3$ can be identified and analysed in n-dimensional lattices. In $\mathbb{E}^4$, the classification of space groups was completed in the work of Brown et al. [4]. Of course, the lattices in $\mathbb{E}^4$ also include fivefold point symmetry; see also [AO1, Table 3.1].

Although applications of this work in high-dimensional crystallography were not immediately clear, the outcome would gain new weight and recognition in physics with the advent of quasicrystals.

E.4. Aperiodic tilings of the plane

R. Penrose 1974

In mathematical crystallography, the Euclidean space $\mathbb{E}^n$ is tiled without gaps or overlaps by copies of the unit cell of a lattice. The positions of the centres of these copies are given by the set of all lattice translations. A natural generalisation of periodicity is to consider tilings that consist of copies of a finite number of cells. If such a tiling fails to be lattice-periodic, one has to find new ways to introduce long-range order.

R. Penrose [38] proposed such a tiling of the plane with two rhombus tiles, which is known as the Penrose pattern; see Figure E.4.1. The edges of the two tiles have the same length. The angles between the edges of these tiles are multiples of $\pi/5$ and so are adapted to fivefold symmetry. It follows that all the edges in the tiling point in only five directions. This already suggests the presence of fivefold symmetry, at least on average. Of course, the tiles themselves could be arranged into periodic tilings, but Penrose (stimulated by Kepler's attempt) wanted to avoid lattice periodicity. As a local rule for the long-range order, he introduced the concept of *matching rules* (also known as local rules; see [AO1, Sec. 5.7]). The matching rules require that the marked

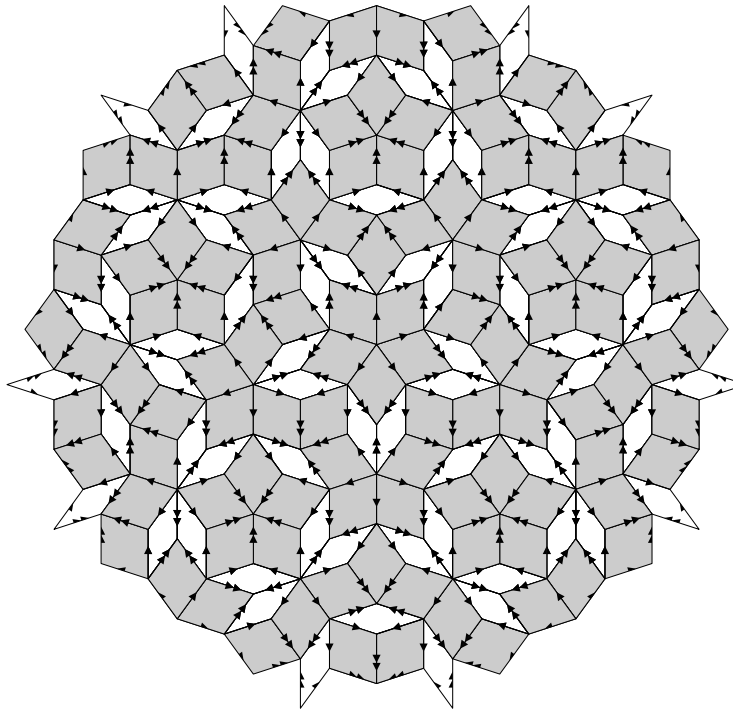

FIGURE E.4.1. Patch of the rhombic Penrose pattern with matching rules (via arrow markers). The two tile shapes are thin or thick rhombuses.

directed edges of adjacent tiles must correspond to one another. Penrose demonstrated a number of interesting properties of his patterns [38, 39].

The paradigm of the Penrose pattern was very appealing to scientists as a template for generalisations of classical crystallography. In particular, one could envisage atoms fixed at specific positions on the rhombus tiles and study the properties of the resulting generalised crystals.

Of particular interest was the question of which other properties of classical crystallography could extend to Penrose patterns. A first question about the Penrose patterns focussed on the implied long-range order. Can any patch of tiles, built according to the local rules, be extended to cover the entire plane? This question has a negative answer: There are finite patches of tiles that obey the matching rules but nevertheless cannot be extended, in some places, without violating the matching rules. Penrose later called this property the non-locality of the pattern [39]. Another problem, which we shall address next, concerned the Fourier and diffraction properties of the Penrose pattern.

E.5. Cells and diffraction of the Penrose pattern

A.L. Mackay 1981/82

A.L. Mackay [32] presented the Penrose pattern as a paradigm for crystallography with fivefold point symmetry. He discussed the planar Penrose rhombus pattern, suggested its two cells as non-periodic generalisations of crystallographic cells, and proposed the name quasi-lattice for the pattern. He also pointed out a three-dimensional generalisation with two rhombohedra whose edges point in the six directions perpendicular to the faces of the regular dodecahedron. He demonstrated in [32, Fig. 8] that these rhombohedra can build Kepler's triacontahedron.

In [33], Mackay posed the question what diffraction would result if one placed scatterers on the vertices of a Penrose pattern. By an optical transform of circular obstacles, placed at vertex positions of a patch of a Penrose pattern, he arrived at a diffraction pattern governed by sharp peaks with intensities whose distribution exhibited tenfold point symmetry. Mackay's result strongly suggested that Penrose's generalisation of crystals shares a pure point diffraction spectrum with classical crystals. Pure point diffraction is the classical basis of structure determination by Fourier analysis, as explained in Section E.1.

E.6. Quasiperiodicity and Fourier modules from higher-dimensional lattice embeddings

H. Bohr 1925

Back in the year 1925, in part II of two papers [2] devoted to a careful mathematical analysis of almost periodicity, H. Bohr explored the notion of quasiperiodicity; see pp. 111–117, pp. 137–140 and pp. 160–162 in [2]. He considered a lattice Γ in Euclidean space $\mathbb{E}^n$ of dimension $n > 1$ and periodic functions f^{p} on this space. His approach can be described as follows. He introduced a decomposition of Euclidean space $\mathbb{E}^n = \mathbb{E}^m_{\parallel} \oplus \mathbb{E}^{n-m}_{\perp}$ into two orthogonal subspaces, $\mathbb{E}^m_{\parallel} \perp \mathbb{E}^{n-m}_{\perp}$, chosen such that $\mathbb{E}^m_{\parallel}$ was irrational relative to the lattice Γ. Here, irrationality meant that, if $\mathbb{E}^m_{\parallel}$ is translated by a vector t so as to intersect with a lattice point P, the intersection of the shifted subspace with the set of all lattice points contains only P, that is, $(\mathbb{E}^m_{\parallel} + t) \cap \Gamma = P$. The Fibonacci tiling, see section E.7 below, provides one of the simplest examples of such an irrational section.

Bohr then analysed a periodic function f^{p} on $\mathbb{E}^n$ with its domain restricted to the subspace $\mathbb{E}^m_{\parallel}$. He showed that this restriction has quasiperiodic properties. Moreover, he considered the Fourier series of f^{p} and analysed the Fourier transform of a function restricted to the irrational parallel subspace.

His finding can be expressed in terms of the lattice Γ^{R} in Fourier k-space that is reciprocal to the original lattice $\Gamma \subset \mathbb{E}^n$. If one projects the points of the reciprocal lattice to the parallel k-subspace $\mathbb{E}^m_{\parallel}$, the countable and non-continuous set of these projections carries the Fourier coefficients of the quasiperiodic function. This set of projected reciprocal lattice points forms what, in mathematical terminology, is called a $\mathbb{Z}$-*module*. By construction, its points can be related in $\mathbb{E}^m_{\parallel}$ by integer linear combinations of basis vectors of the reciprocal lattice, projected to this subspace. In contrast to the reciprocal lattice points of periodic crystals, the points belonging to the quasiperiodic module are countable (and hence do not form a continuum) but are dense, that is, they come arbitrarily close to other points of the module.

The ingredients of Bohr's description of quasiperiodic functions were then a periodic lattice $\Gamma \subset \mathbb{E}^n$ and an irrational subspace $\mathbb{E}^m_{\parallel}$ with $1 \leqslant m < n$. On this basis, Bohr provided a countable and non-continuous Fourier module whose points carried the Fourier coefficients for quasiperiodic functions.

The Fibonacci paradigm, discussed in the next section, provides a simple example of Bohr's theory. For general applications of Bohr's ideas, there remained a problem: The points of a lattice form only a countable subset of $\mathbb{E}^n$ leaving ample gaps for irrational subspaces. Among the infinite set of irrational subspaces, what guideline can lead to a significant choice?

E.7. Scaling and the square lattice

Fibonacci 1202 and Lothaire 1983

In 1202, Leonardo da Pisa (also known as Fibonacci) published his handwritten monograph *Liber abaci* in Pisa. In this work, he presented the integer sequence, now widely known as the Fibonacci numbers, defined recursively by $f_1 = f_2 = 1$ together with

$$f_{n+1} \;=\; f_n + f_{n-1}, \tag{E.7.1}$$

so that

$$f_1 = f_2 = 1,\ f_3 = 2,\ f_4 = 3,\ f_5 = 5, \ldots$$

Fibonacci numbers appear in mathematical combinatorics, see M. Lothaire [31, p. 10] and references therein, as follows. Consider an alphabet $A = \{a, b\}$ and words formed recursively by concatenation,

$$\begin{aligned} &w_{n+1} \;=\; w_n w_{n-1}, \quad n \geqslant 2, \\ &w_1 = b,\ w_2 = a,\ w_3 = ab,\ w_4 = aba,\ w_5 = abaab, \ldots \end{aligned} \tag{E.7.2}$$

Counting the number of letters in successive words, with $|w_n|$ the length of w_n, one finds

$$|w_1| = |w_2| = 1, \quad |w_{n+1}| = |w_n| + |w_{n-1}| = f_{n+1}. \tag{E.7.3}$$

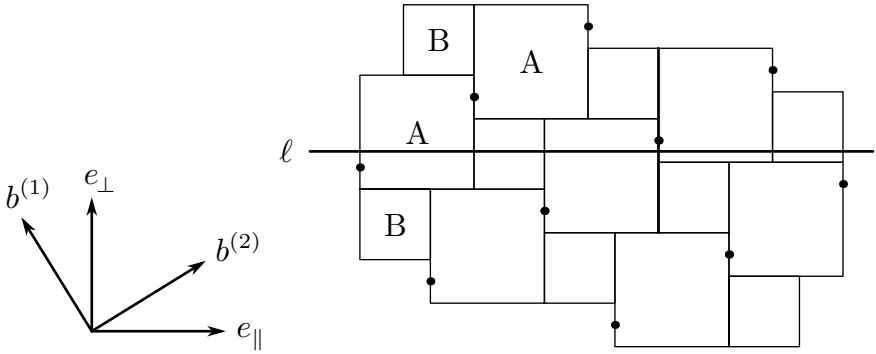

FIGURE E.7.1. Illustration of the Fibonacci tiling as obtained from the square lattice. The black dots denote the points of the square lattice. The two squares A and B give a periodic tiling of the plane. The Fibonacci matrix M_{F} determines the scalings in the two perpendicular directions $e_\parallel$ and $e_\perp$. A generic line ℓ parallel to $e_\parallel$ intersects the two squares in two intervals of length ratio τ. This sequence of intervals generates the Fibonacci tiling on the line, here with the word *abaab*; compare Eq. (E.7.2).

So, the length of each word is a Fibonacci number. From the relative frequencies of the letters a and b in these 'Fibonacci words', one can easily prove (by a standard limit argument) that the infinite Fibonacci words cannot be periodic. These words can be converted into an aperiodic tiling by interpreting the letters a and b as intervals on the line of length τ and 1, respectively, where $\tau = \frac{1}{2}\left(1+\sqrt{5}\right)$ is the golden mean; compare [AO1, Ex. 4.6] for further details.

The recursive construction in Eq. (E.7.2) is the first approach to the Fibonacci tiling. In a second step, we now relate the Fibonacci tiling to Bohr's theory of quasiperiodic functions. For this, we follow the exposition of [26, pp. 311–312] and define the substitution matrix

$$M_{\mathrm{F}} \;=\; \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}. \tag{E.7.4}$$

This matrix belongs to the group $\mathrm{GL}(2,\mathbb{Z})$ with integer matrix elements and determinant ± 1. Computation of the powers of this matrix relates them to the Fibonacci numbers by

$$M_{\mathrm{F}}^n \;=\; \begin{pmatrix} f_{n+1} & f_n \\ f_n & f_{n-1} \end{pmatrix}, \quad \det(M_{\mathrm{F}}^n) = (-1)^n. \tag{E.7.5}$$

The two eigenvalues of M_{F} are

$$\lambda_1 \;=\; -\tau^{-1} = 1-\tau, \quad \text{and} \quad \lambda_2 \;=\; \tau \;=\; \frac{1+\sqrt{5}}{2}. \tag{E.7.6}$$

The eigenvectors are derived from the equation

$$BM_{\mathrm{F}}B^{-1} = \begin{pmatrix} -\tau^{-1} & 0 \\ 0 & \tau \end{pmatrix}, \tag{E.7.7}$$

as the two orthonormal column vectors $b^{(1)}$ and $b^{(2)}$ of the matrix

$$B = \begin{pmatrix} -\sqrt{\frac{-\tau+3}{5}} & \sqrt{\frac{\tau+2}{5}} \\ \sqrt{\frac{\tau+2}{5}} & \sqrt{\frac{-\tau+3}{5}} \end{pmatrix}. \tag{E.7.8}$$

The two vectors thus emerge from the initial orthogonal basis, see the left panel of Figure E.7.1, by an application of the matrix B. Writing Eq. (E.7.7) as

$$\begin{pmatrix} -\tau^{-1} & 0 \\ 0 & \tau \end{pmatrix} B = B \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \tag{E.7.9}$$

suggests the following interpretation. The basis vectors $b^{(1)}$ and $b^{(2)}$ span a square lattice. The right action of M_{F} on B, given on the right-hand side of Eq. (E.7.9), transforms lattice points into lattice points via integer linear combinations of the basis vectors $b^{(1)}$ and $b^{(2)}$. The left-hand side shows that this is a scaling of $b^{(1)}$ and $b^{(2)}$ by the factors λ_1 and λ_2, respectively.

We can now combine this result with Bohr's theory of quasiperiodic functions as follows. The orthogonal basis vectors $e_{\parallel} = (1,0)^T$ and $e_{\perp} = (0,1)^T$ determine two irrational, orthogonal directions through the square lattice and provide one-dimensional irrational subspaces $\mathbb{E}_{\parallel}$ and $\mathbb{E}_{\perp}$. With respect to these directions, the original matrix M_{F} becomes diagonal. One can construct [26] a new periodic tiling of $\mathbb{E}^2$ by two squares whose boundaries are parallel to the directions of these subspaces; see Figure E.7.1.

Now, a generic line ℓ parallel to $e_{\parallel}$ intersects these two squares in two intervals. These intervals (resp. their endpoints) belong to a module on the line. Their length ratio is the golden mean τ and the tiling on the line ℓ is a Fibonacci tiling. A parallel scaling by a factor τ maps endpoints of intervals to endpoints. So, the Fibonacci tiling has a scaling symmetry and displays a cell structure. The scaling symmetry selects a particular one-dimensional irrational subspace in the square lattice, and hence, by Bohr's theory, becomes a source of quasiperiodicity. Similar lattice scalings by powers of τ appear in lattices of $\mathbb{E}^4$ and $\mathbb{E}^6$ with fivefold and icosahedral symmetry, respectively. These scalings underlie the notions of inflation and self-similarity; compare [AO1, Ch. 6] for further examples.

It follows from Bohr's theory that the Fibonacci tiling is quasiperiodic and hence has a countable, dense Fourier module; see [AO1, Sec. 9.4.1] for an explicit calculation in a slightly different setting.

E.8. Harmonious sets

Y. Meyer 1970/72

In [34, 35], Y. Meyer, starting from a mathematical study of harmonic analysis on locally compact Abelian groups, introduced certain discrete point sets, which he called harmonious sets. After the discovery of quasicrystals, it was realised that these harmonious or Meyer sets generalise the notion of lattices to general aperiodic structures, and so provide a mathematical framework including and generalising quasicrystals.

Of the seven equivalent characterisations of Meyer sets given by R.V. Moody [36, pp. 403–441], we mention only a geometric one here. One begins with a Delone set $\varGamma \subset \mathbb{R}^d$, defined as a relatively dense and uniformly discrete set. This Delone set is a Meyer set if there is a finite set $F \subset \mathbb{R}^d$ such that the set of differences obeys $\varGamma - \varGamma = \varGamma + F$. One clearly recognises the generalisation of the notion of a lattice, where the set of differences would result in $F = \{0\}$.

Moody [36, pp. 403–441] gives a detailed mathematical account of Meyer's harmonious sets in the light of our present knowledge of aperiodic structures. The broader field of mathematics of aperiodic structures is the subject of the volume [36], edited in 1997 by Moody; see also [AO1].

E.9. Fourier analysis of incommensurate and modulated crystals

A. Janner and T. Janssen 1977

A first and successful application of Bohr's theory to the crystallography of quasiperiodic functions was made by A. Janner and T. Janssen [16, 17], based on previous work of P.M. de Wolff [6]. The idea was to describe the so-called incommensurate and modulated structures found in certain classes of crystals, by the extension of three-dimensional space to a superspace equipped with a superlattice. The extra dimensions are used to describe the incommensuration and modulation.

The introduction of a reciprocal Fourier superspace, and its projection to the usual Fourier space, then provided, in addition to the usual diffraction pattern, a pattern of satellite diffraction peaks whose structure encodes the specific nature of the incommensuration or modulation. Here, the Fourier analysis beyond periodicity was developed, extended and applied in the spirit of Bohr's concept of quasiperiodicity; see [AO1, Sec. 9.2.6] for some examples.

E.10. The quasiperiodic Penrose pattern in two dimensions derived from a lattice

N.G. de Bruijn 1981

From a mathematical perspective, the first analysis of the Penrose pattern in terms of a lattice embedding into four-dimensional space $\mathbb{E}^4$ was presented by de Bruijn [5]. His choice of four dimensions was guided by the wish to incorporate fivefold point symmetry: The Euclidean space $\mathbb{E}^4$ has the lowest dimension that allows for a lattice embedding with fivefold point symmetry. If one examines the action of the cyclic group C_5 on $\mathbb{E}^4$, via a real representation, one finds two orthogonal invariant subspaces of dimension 2. The unique invariant subspace $\mathbb{E}^2_\parallel$ of $\mathbb{E}^4$ in which the cyclic group generator acts as a rotation by an angle $2\pi/5$ is the natural choice of $\mathbb{E}^2_\parallel$ for a quasiperiodic function. This subspace has the property of being irrational with respect to the (properly chosen) lattice in $\mathbb{E}^4$.

The next task of de Bruijn was to identify the Penrose rhombus tiles as projections. We take the liberty of describing his findings in the terminology of a later analysis of the same lattice in $\mathbb{E}^4$ as given in [1]. The lattice provides two tilings of $\mathbb{E}^4$ by 4-polytopes. One is a tiling by Voronoi polytopes, which are the Wigner–Seitz cells of the lattice, centred at the lattice points. The second, dual tiling is given by so-called Delone polytopes, centred at the vertices of the Voronoi domains. His geometric view allowed de Bruijn to identify the Penrose rhombus tiles with what is denoted in [1] as the projections of two-dimensional boundaries of the Delone cells. De Bruijn introduced a so-called *pentagrid* for the construction of a Penrose rhombus tiling by projection; see also [AO1, Sec. 7.5.2].

De Bruijn's contribution to the theory of quasicrystals advanced the field considerably. His construction of an irrational lattice embedding into four-dimensional space related the planar Penrose tiling construction to the theory of Bohr. This construction showed that the requirement of fivefold point symmetry uniquely determines the irrational subspace required by Bohr's theory. So, the fivefold point symmetry indeed promised to be a gateway to a new type of long-range order.

When combined with Bohr's theory, it followed from de Bruijn's construction that the Fourier transform of a Penrose pattern can be described by a dense module of sharp diffraction points, whose positions are projections of the reciprocal lattice points into a two-dimensional Fourier k-subspace. This consequence confirmed that Mackay's conjecture of sharp diffraction peaks from a Penrose pattern had a strict mathematical basis.

E.11. Icosahedral tilings in three dimensions

P. Kramer 1982/84

The pentagram had led to the Penrose paradigm of a quasiperiodic planar tiling in two dimensions. However, crystals in physics are phenomena in three dimensions. The counterpart of the pentagram is the icosahedron, whose point symmetry is forbidden in three-dimensional lattices. This now prompted, in three-dimensional space, the quest for tiles and tilings with forbidden icosahedral point symmetry. The first (recursive) and the second (lattice) approach discussed in Section E.7 for the Fibonacci tiling looked promising. Kramer [23] constructed a first set of seven elementary convex polyhedral tiles with two properties, namely

(i) copies of them could be packed into a regular dodecahedron;

(ii) copies of the seven tiles could be packed into polyhedra of the same seven shapes, but scaled by a factor which was the third power of the golden mean $\tau = \frac{1}{2}\big(1 + \sqrt{5}\,\big)$.

It was then clear that, by repeated application of this self-similar scaling, any region of three-dimensional space could be covered by a tiling of the seven elementary tiles. Mosseri and Sadoc [37] later managed to reduce the number of these tiles from seven to four.

The findings by de Bruijn [5] and by Bohr [2] suggested the following lattice construction for icosahedral quasicrystals.

(1) Find a lattice in $\mathbb{E}^n$ that is invariant under the action of the icosahedral group Y;

(2) Moreover, identify a subspace $\mathbb{E}^3_{\parallel} \subset \mathbb{E}^n$ of dimension 3 that is invariant under the action of Y.

Kramer and Neri [28] showed that the hypercubic lattice in six-dimensional space was compatible with icosahedral point symmetry, and moreover provided a unique three-dimensional subspace that is invariant under the icosahedral rotation group Y in its standard three-dimensional representation.

By considering the Voronoi 6-polytopes of the hypercubic lattice in $\mathbb{E}^6$ and their three-dimensional boundaries, both projected to the parallel space $\mathbb{E}^3_{\parallel}$ with icosahedral symmetry, Kepler's triacontahedron emerged from the Voronoi polytope, and rhombohedra in two shapes from the three-dimensional boundaries. This icosahedral tiling is thus built exactly from the tiles considered by Mackay [33]; see Figure E.11.1 as well as [AO1, Sec. 7.4]. As was found out later, Kowalewski, in his 1938 book on recreational mathematics [22], had already described Kepler's triacontahedron and the two rhombohedra as icosahedral projections of the hypercube in six dimensions and its boundaries.

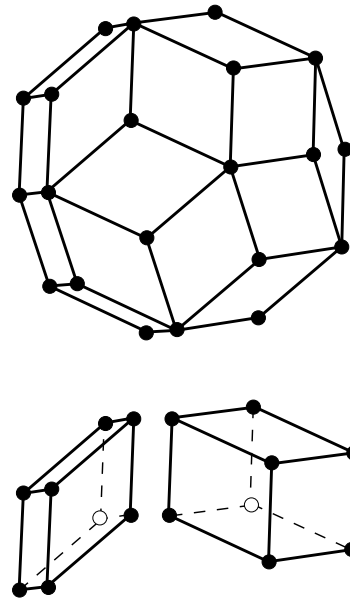

FIGURE E.11.1. The icosahedral projection to $\mathbb{E}^3_{\parallel}$ of the hypercubic Voronoi polytope in $\mathbb{E}^6$ is Kepler's triacontahedron. The three-dimensional boundaries of the hypercube project into a thin and a thick rhombohedron.

The work by Kramer and Neri generated the first paradigm of a quasicrystal with icosahedral point symmetry in three-dimensional space. Combined with Bohr's general theory, a diffraction analysis on an appropriate icosahedral Fourier module could be devised. A generalisation of de Bruijn's planar pentagrid to a hexagrid in three dimensions provided [24, 27, 25] the construction of an icosahedral tiling from the two rhombohedral tiles. Duality in the high-dimensional lattice, in analogy of what is shown in Figure E.1.1, plays a major role.

The enigma of the pentagram was finally solved. Fivefold and icosahedral symmetry were back on their way into physics.

E.12. Discovery of iscosahedral quasicrystals

D. Shechtman, D. Gratias, I. Blech and J.W. Cahn 1984

In the previous sections, we surveyed the theoretical approaches to quasicrystals prior to their experimental discovery.

In 1984, D. Shechtman, D. Gratias, I. Blech and J.W. Cahn [44] announced the discovery of quasicrystals — a new type of matter that exhibited a diffraction pattern with sharp peaks of icosahedral point symmetry. This

discovery implied that atomic matter could organise itself according to the new paradigm of quasiperiodic long-range order. An international workshop at Les Houches in 1986 [13] brought together many protagonists of quasicrystal theory with D. Shechtman and his colleagues. A brief review along similar lines as given here can be found in J.W. Cahn's epilogue [15, pp. 807–810] to the 5th International Conference on Quasicrystals, Avignon 1995.

E.13. Postscriptum

D. Levine and P.J. Steinhardt 1984
H.Q. Ye and K.H. Kuo 1984
T. Ishimasa, H.-U. Nissen and Y. Fukano 1985
A. Katz and M. Duneau 1986
B. Grünbaum and G.C. Shephard 1987

The extraordinary development of quasicrystals after 1984, both on the experimental and the theoretical level, is another story which we shall not tell here. We finish this overview with a brief summary of theoretical and experimental work that was published shortly after the experimental discovery of quasicrystals.

In 1984, D. Levine and P.J. Steinhardt [30] devised a construction method for non-periodically ordered structures based on the Fibonacci sequence, and proposed the name *quasicrystals* for such structures. Two years later, A. Katz and M. Duneau [18] developed projection methods for the construction of icosahedral tilings by rhombohedra. The geometry of tilings was comprehensively described in a monograph written in 1987 by B. Grünbaum and G.C. Shephard [10].

Expanding the field of quasicrystals on the experimental side, in 1984 H.Q. Ye and K.H. Kuo [48] studied quasicrystals with layers of forbidden tenfold point symmetry. In 1985, T. Ishimasa, H.-U. Nissen and Y. Fukano [14] prepared structures with (Ni,Cr) atomic composition and non-crystallographic twelvefold point symmetry.

Since 1986, the broad development of quasicrystal preparation, structure analysis and new physical properties have been manifest in the Proceedings of International Conferences on Quasicrystals, 1986 in Les Houches (France) [13], 1989 in Vista Hermosa (Mexico) [47], 1992 in St Louis (USA) [21], 1995 in Avignon (France) [15], 1997 in Tokyo (Japan) [45], and 1999 in Stuttgart (Germany) [9]. To date, this conference series is still continuing.

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